

# Theory of the 1-point PDF for incompressible Navier-Stokes fluids

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Fundamental aspects of fluid dynamics are related to construction of statistical models for incompressible Navier-Stokes fluids. The latter can be considered either *deterministic* or *stochastic*, respectively for *regular* or *turbulent flows*. In this work we claim that a possible statistical formulation of this type can be achieved by means of the 1-point (local) velocity-space probability density function (PDF,  $f_1$ ) to be determined in the framework of the so-called inverse kinetic theory (IKT). There are several important consequences of the theory. These include, in particular, the characterization of the initial PDF [for the statistical model  $\{f_1, \Gamma\}$ ]. This is found to be generally non-Gaussian PDF, even in the case of flows which are regular at the initial time. Moreover, both for regular and turbulent flows, its time evolution is provided by a Liouville equation, while the corresponding Liouville operator is found to depend only on a finite number of velocity moments of the same PDF. Hence, its time evolution depends (functionally) solely on the same PDF. In addition, the statistical model here developed determines uniquely both the initial condition and the time evolution of  $f_1$ . As a basic implication, the theory allows the *exact construction of the corresponding statistical equation for the stochastic-averaged PDF* and the *unique representation of the multi-point PDF's* solely in terms of the 1-point PDF. As an example, the case of the reduced 2-point PDF's, usually adopted for the statistical description of NS turbulence, is considered.

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## 1 - INTRODUCTION

The description of fluids, and more generally of continua, is based on the introduction of a suitable set of *fluid fields*  $\{Z\}$  which define the state of each fluid and obey, by assumption, a well-posed set of PDE's denoted as *fluid equations*. The formulation appropriate for an incompressible Navier-Stokes (NS) fluid - based on the so-called incompressible NS equations (INSE) - is recalled in Appendix A, together with the basic notations and definitions here adopted. The fluid equations, the fluid fields and the related initial and boundary conditions, are considered either as *deterministic* or *stochastic*, respectively for *regular* or *turbulent flows* (see Appendix A, Subsections A.2 and A.3).

The statistical treatment of fluids usually adopted for turbulent flows (which may be invoked, however, to describe also regular flows) consists, instead, in the introduction of appropriate axiomatic approaches denoted as *statistical models*. These are sets  $\{f, \Gamma\}$  formed by a suitable probability density function (PDF) and a phase-space  $\Gamma$  (subset of  $\mathbb{R}^n$ ) on which  $f$  is defined. By definition, a statistical model  $\{f, \Gamma\}$  of this type must permit the representation, via a suitable mapping

$$\{f, \Gamma\} \Rightarrow \{Z\}, \quad (1)$$

of the *complete set* (or more generally only of a *subset*) of the *fluid fields*  $\{Z\} \equiv \{Z_i, i = 1, n\}$  which define the state of the same fluids. Their construction involves, besides the specification of the phase space ( $\Gamma$ ) and the *probability density function* (PDF)  $f$ , the identification of the functional class to which  $f$  must belong, denoted

as  $\{f\}$ . As a consequence, the fluid fields  $Z_i \in \{Z\}$  are expressed in terms of suitable functionals (called *moments*) of  $f$ . In the case of an incompressible (and isentropic) Navier-Stokes fluid (INSF) the latter are identified with  $\{Z\} \equiv \{\mathbf{V}, p, S_T\}$ ,  $\mathbf{V}$  and  $p$  indicating respectively the fluid velocity, the fluid pressure, both assumed strong solutions the incompressible Navier-Stokes equations (INSE), and  $S_T$  the constant thermodynamic entropy. As an alternative,  $p$  can be replaced by the kinetic pressure  $p_1$ , to be suitably defined [see subsequent Eq.(27)].

Goal of this paper is to propose a *statistical model* for incompressible NS fluids, described by INSE, which is simultaneously (a) *unique*, (b) *statistically complete* and (c) *closed*. While the precise meaning of these statements, in particular the relationship (1), will be discussed in detail below, we anticipate that:

- the first condition (uniqueness) imposes that the same PDF and its time evolution should both be uniquely prescribed in terms of *conditional observables* (see related definitions in the Appendix A);
- the second one (statistical completeness; see subsequent Subsection 1D) involves the assumption that the PDF should determine uniquely also a prescribed set of *physical observable* (or rather *conditional observables*), to be suitably defined. The latter include in particular the complete set of fluid fields describing the state of the fluid;
- the third one (closure) includes both *moment-* and *kinetic-closure conditions* (the corresponding definitions are given again in Subsection 1D), involving

- respectively - the requirements that there exists a closed set of fluid equations and that the statistical equation advancing in time the PDF depends only the same PDF, via a finite number of moments (of the PDF).

### 1A - CSM-inspired models for the 1-point Liouville equation

A well-known example of statistical model for incompressible NS fluids is provided by the so-called *statistical hydromechanics* developed originally by Hopf [1] and later extended by Rosen [2] and Edwards [3] (*HRE approach*). This relies on the introduction of the *1-point (or local) velocity-space PDF*,  $f_1$ , to be intended as the conditional PDF of the velocity  $\mathbf{v}$  (*kinetic velocity*) with respect the remaining variables. In the HRE approach these are identified with  $(\mathbf{r}, t)$ , where  $(\mathbf{r}, t) \in \Omega \times I$ , while  $f_1 \equiv f_1(\mathbf{r}, \mathbf{u}, t; Z)$ , with  $\mathbf{u} \equiv \mathbf{v} - \mathbf{V}(\mathbf{r}, t)$  the relative kinetic velocity, is identified with

$$f_H \equiv \delta(\mathbf{v} - \mathbf{V}(\mathbf{r}, t)) \quad (2)$$

(*deterministic PDF*),  $f_H$  denoting the three-dimensional Dirac delta defined in the velocity space  $U \equiv \mathbb{R}^3$ , with  $\mathbf{v}$  belonging to  $U \equiv \mathbb{R}^3$  and  $(\mathbf{r}, t) \in \overline{\Omega} \times I$  (with  $\overline{\Omega}$  denoting the closure of the configuration domain  $\Omega \subseteq \mathbb{R}^3$ ). Hence,  $f_H$  is defined by assumption on the set spanned by the state vector  $\mathbf{x} = (\mathbf{r}, \mathbf{v})$ , i.e.,  $\overline{\Gamma} \equiv \overline{\Omega} \times U$ , with  $\overline{\Gamma}$  denoting the closure of the *restricted phase space*

$$\Gamma \equiv \Omega \times U. \quad (3)$$

It follows that, in this case, only the first two (velocity) moments of  $f_1$ , corresponding to  $G = 1, \mathbf{v}$ , are actually prescribed in terms of the fluid fields and read

$$\int_U d^3 \mathbf{v} G f_H(\mathbf{r}, \mathbf{u}, t; Z) = 1, \mathbf{V}(\mathbf{r}, t). \quad (4)$$

Goal of the HRE approach in the case of turbulent flows is actually to predict

$$\langle f_1(\mathbf{r}, \mathbf{u}, t; Z) \rangle \equiv \langle f_H(\mathbf{r}, \mathbf{u}, t; Z) \rangle, \quad (5)$$

the brackets "⟨ · ⟩" denoting an ensemble average, to be suitably prescribed, over the possible realizations of the fluid [6]. Its definition, however, is not unique. For example, in the case of the so-called stationary and isotropic turbulence [4] this is usually defined so that - by assumption - it commutes with all the differential and integral operators (respectively,  $\frac{\partial}{\partial t}, \nabla, \nabla^2$  and  $\int_U d^3 r, \int_U d^3 v$  and  $\int_{\Omega} d^6 x$ ) appearing in the NS operator [see Eq.(94), in Appendix A]. As an alternative, as discussed elsewhere [13], ⟨ · ⟩ can also be identified with the stochastic-averaging operator (106) defined in Appendix A.

Nevertheless, in the HRE approach  $\langle f_H \rangle$  is not directly determined. Rather, it is replaced by a suitable functional of  $\langle f_H \rangle$ ,  $\phi$ , which obeys a suitably-prescribed functional-differential equation (the so-called " $\phi$  equation" [1]). The problem of the construction of an equivalent evolution (or so-called "transport") equation for  $\langle f_H \rangle$  has been investigated by several authors (see, for example, Dopazo [5] and Pope [6]). The construction of its formal solution is due to Monin [7] and Lundgren [8] (*ML approach*; see also Monin and Yaglom, 1975 [9] and therein cited references). However, alternative (approximate) statistical approaches are known, such as the GLM (generalized Langevin model; due to Pope [10]). All of them typically rely on the assumption of the existence of a suitable underlying *phase-space classical dynamical system* which evolves in time the state vector  $\mathbf{x} = (\mathbf{r}, \mathbf{v})$ , namely the flow

$$T_{t_o, t} : \mathbf{x}_o \rightarrow \mathbf{x}(t) = T_{t_o, t} \mathbf{x}_o \quad (6)$$

generated by an initial value problem of the type

$$\begin{cases} \frac{d\mathbf{x}}{dt} = \mathbf{X}(\mathbf{x}, t; Z), \\ \mathbf{x}(t_o) = \mathbf{x}_o. \end{cases} \quad (7)$$

Here the notation is standard [11, 12]. Thus,  $T_{t_o, t}$  is the evolution operator generated by

$$\mathbf{X}(\mathbf{x}, t; Z) = \{\mathbf{v}, \mathbf{F}\}, \quad (8)$$

$\chi(\mathbf{x}_o, t_o, t)$  being the solution of the initial-value problem and  $\mathbf{F}(\mathbf{x}, t; Z)$  a vector field (denoted as *mean-field force*) to be suitably prescribed. The definitions of the PDF and of its functional class  $\{f_1\}$  depend on the type of relationship established between the fluid fields and the PDF, to be prescribed in some suitable sense. In CSM-inspired statistical models this is realized by means of a PDF,  $f_1$ , which is assumed to satisfy the corresponding *1-point Liouville equation* - here denoted as *inverse kinetic equation* (IKE [11, 12]) - of the form

$$L(\mathbf{r}, \mathbf{v}, t; f_1) f_1(\mathbf{r}, \mathbf{u}, t; f_1) = 0. \quad (9)$$

Here  $L(\mathbf{r}, \mathbf{v}, t; f_1)$  denotes the Liouville streaming operator

$$\begin{aligned} L(\mathbf{r}, \mathbf{v}, t; f_1) \cdot &\equiv \frac{\partial}{\partial t} \cdot + \frac{\partial}{\partial \mathbf{x}} \cdot \{\mathbf{X}(\mathbf{x}, t; Z) \cdot\} \equiv & (10) \\ &\equiv \frac{\partial}{\partial t} \cdot + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \cdot + \frac{\partial}{\partial \mathbf{v}} \cdot \{\mathbf{F}(\mathbf{x}, t; f_1) \cdot\}, \end{aligned}$$

while the vector field  $\mathbf{F}$  is generally to be assumed functionally dependent on  $f_1$ . In particular, in the HRE and ML approaches this is obtained by invoking the position

$$\mathbf{F} \equiv \mathbf{F}_H, \quad (11)$$

with  $\mathbf{F}_H$  denoting the total fluid force density acting on each fluid element [see Eq.(96) in the Appendix] and identifying  $f_1$  with the particular solution

$$f_1 = f_H \quad (12)$$

[with  $f_H$  defined by Eq.(2)]. Hence in this case  $\{f_1\}$  is manifestly the functional class of distributions of the form (2).

The HRE and ML approaches, both characterized by the same statistical model  $\{f_H, \Gamma\}$  (*HRE-ML statistical model*), belong actually to a more general class of statistical models inspired by Classical Statistical Mechanics (CSM) (see also Sec.2).

In particular, this concerns the representation of all the relevant dynamical variables in terms of *hidden variables* [13, 14] (see Appendix A). By definition they denote a suitable set of independent variables  $\alpha = \{\alpha_i, i = 1, k\} \in V_\alpha \subseteq \mathbf{R}^k$ , with  $k \geq 1$ , which cannot be known deterministically, i.e., are not observable. In the context of turbulence theory these variables are necessarily stochastic. This means that they are characterized by a suitable *stochastic probability density*  $g$  defined on  $V_\alpha$  (see definitions and related discussion in Appendix A, Subsection A.2), while the ensemble average  $\langle \cdot \rangle$  [defined in Eq.(5)] can be identified with the stochastic-averaging  $\langle \cdot \rangle_\alpha$  defined by Eq.(106) [see Appendix A]. Hence, for turbulent flows the fluid fields - together with the PDF  $f_1$  and the vector field  $\mathbf{F}(\mathbf{x}, t; Z)$  appearing in Eqs.(8) and (9) - admit a representation of the form [13, 14]

$$\begin{cases} \{Z\} = \{Z(\mathbf{r}, t, \alpha)\} \\ f_1 = f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z) \\ \mathbf{F} = \mathbf{F}(\mathbf{x}, t, \alpha; Z) \end{cases} \quad (13)$$

to be defined in terms of a set of hidden variables  $\alpha$  and a stochastic model  $\{g, V_\alpha\}$  (see again Appendix A, Subsection A.2). Hence,  $\{Z\}$ ,  $f_1$  and  $\mathbf{F}(\mathbf{x}, t; Z)$  are necessarily *non-observable*. Nevertheless, if we assume that the fluid fields  $\{Z\}$  are uniquely-prescribed ordinary functions of  $(\mathbf{x}, t, \alpha)$  defined for all  $(\mathbf{x}, t, \alpha) \in \bar{\Gamma} \times I \times V_\alpha$ , it follows that they can still be considered *conditional observables* (see Appendix A, Subsection A.1). Similar conclusions apply to  $f_1$ , and to the vector field  $\mathbf{F}(\mathbf{x}, t; Z)$  as well.

## 1B - The Closure problem

Based on these requirements [the positions defined by Eqs.(11) and (12)], in turbulence theory, i.e., when the fluid fields  $\{Z\}$  are considered as stochastic functions, usually the statistical description involves the construction of an infinite set of *continuous* many-point PDF's which obey a hierarchy of statistical equations, the so-called ML (Monin-Lundgren [7, 8]) hierarchy. Therefore in this case the statistical model actually involves the identification of  $\{f\}$  with the functional class of the many-point PDF's. As proven by Hosokawa [15], the problem can be formulated in an equivalent way in the framework of the HRE approach, yielding the well-known Hopf  $\phi$  functional-differential equation.

To date, the search of possible exact "closure conditions" for the ML hierarchy (or *closure problem*) - or equivalent, of exact solutions of the HRE approach - remains one of the major unsolved theoretical problems in fluid dynamics. For the ML-approach, this involves in principle the construction of statistical models which should be characterized by a finite number of (multi-point) PDF's, i.e., determined in such a way that the time evolution of the fluid fields can be uniquely determined in terms of them. In practice the program of constructing theories of this type, and holding for arbitrary fluid fields, is still open due to the difficulty of preserving the full consistency with the fluid equations. In fact, it is well known that many of the customary statistical models adopted in turbulence theory - which are based on closure conditions of various type (see for example Monin and Yaglom [9] 1975 and Pope, 2000 [6]) - typically reproduce at most only in some approximate (i.e., asymptotic) sense the fluid equations.

In particular, an interesting related issue is that posed by the determination of the form of the 1-point PDF. In decaying isotropic turbulence, according to some authors (see in particular Batchelor [4]) this is predicted as *almost-Gaussian*. Although others, based on the adoption of suitable model dynamical systems for NS turbulence (Falkovich and Lebedev [16] and Li and Menevau [17]), have pointed that the tails of the 1-point PDF might exhibit a strongly *non-Gaussian behavior*, according to more recent investigations (Hosokawa [18]) there seems to be still insufficient experimental evidence for a generalized behavior of this type, at least in the case of homogeneous turbulence.

The basic difficulty is, however, related to the proper formulation of a rigorous theory for the 1-point PDF holding for arbitrary NS fluids. In this reference, in particular, an important issue is related to the quest of a possible *exact statistical evolution equation* for the 1-point PDF [14], *holding both for deterministic and stochastic fluid equations*, which is capable of yielding the correct fluid fields and holds for arbitrary initial and boundary conditions of the relevant related physical observables (or, respectively, conditional observables).

This refers, in particular, to the subset of statistical models  $\{f, \Gamma\}$  in which the PDF  $f$  is considered as an ordinary function.

An example is provided by IKT [11, 12] in which the 1-point PDF obeys by construction, both for regular fluids (i.e., deterministic) and turbulent (i.e., stochastic) fluid fields, an IKE of the form (9).

This result raises the interesting question whether, in some suitable setting, i.e., *for appropriate statistical models* and in particular in the case in which  $\{f\}$  is a set of ordinary functions, the closure problem can actually be solved. In this regard, there are actually two possible routes which seem currently available:

- *the first route:* for a prescribed statistical model  $\{f, \Gamma\}$  it involves the search of possible finite subset of statistical equations (formed by the  $s$  equations for the PDF's,  $f_n$ , having  $n \leq s$  and  $s$  finite) which define a closed set of equations;
- *the second route:* is based on the search of possible alternative statistical models  $\{f, \Gamma\}$ , based on the hidden-variable representation (13) and *mathematically equivalent to the complete set of fluid equations for INSF, for which  $\Gamma$  coincides with the restricted phase-space and the PDF, identified with the 1-point (or local) PDF  $f_1$ , satisfies an IKT of the type defined by (9), in which the mean-field force  $\mathbf{F}$  depends functionally only from  $f_1$ , via suitable moments of the PDF. Statistical models of this type (in which the evolution operator depends only on  $f_1$ , via its moments) are usually said to satisfy a kinetic closure condition.*

The first approach, by far the most popular one in the literature and adopted by several authors for the construction of approximate closure models of the ML hierarchy, poses nevertheless - as indicated above - a problem of formidable difficulty.

Instead, a possible candidate for statistical models of the second type, adopting the hidden-variable representation (13), is already known [13, 14]. It is provided by the 1-point PDF  $f_1$  which characterizes the IKT for an incompressible NS fluid [11, 12]. In this case the PDF can always be required to be also a *velocity-space probability density*, i.e. to satisfy the normalization  $\int_U d^3\mathbf{v} f_1 = 1$ .

In both cases, however, it must be stressed that 'a priori' the definition of relevant statistical model still remains essentially arbitrary. This concerns, besides the choice of the phase-space  $\Gamma$  (only for the first route) and of the functional class  $\{f_1\}$  to which the PDF belongs, also the definition of the set of moments to be associated to the fluid fields  $\{Z\}$ . In particular, in IKT in principle the definition of  $f_1$  is non-unique because higher-order moments of  $f_1$  may be still undetermined. In addition  $f_1$  - even if assumed as an ordinary function - still remains by definition *non-observable*.

## 1C - Physical realizability conditions on the 1-point PDF

In reference to statistical models based on  $f_1$ , such as the IKT model, a natural question arises, i.e., whether the arbitrariness in their definition can be used, *by proper prescription on its functional class  $\{f_1\}$ , to determine it uniquely consistent not only with INSE but also with the relevant physical observables* (or conditional observables). In such a case  $f_1$  might, in particular, be viewed as a *conditional observable* too.

An important preliminary task to accomplish is to establish the relationship of  $f_1$  with the fluid fields. More precisely, here we wish:

A) *to assess whether - besides the complete set of fluid fields - the PDF is possibly related to additional observables or conditional observables. This information, in fact, might provide an effective constraint on the functional class of the initial PDF - evaluated at the initial time ( $t = t_o$ ) -  $\{f_1\}_{r_o}$ ;*

B) *to determine whether, for suitable fluid fields, there exists a deterministic limit for  $f_1$ , namely for which it is a Dirac delta of the type (12). Such a limit would manifestly provide a constraint on the functional class  $\{f_1\}$ .*

Let us point out that for both problems a simple solution actually exists.

### 1C.a - The 1-point velocity-frequency density function

In particular, regarding the observable, here we claim that it can be identified with the *configuration-space average* of 1-point PDF,  $f_1(t) \equiv \langle f_1(\mathbf{r}, \mathbf{v}, t, \alpha; Z) \rangle_\Omega$ , namely  $\langle \cdot \rangle_\Omega$ ,  $\langle \cdot \rangle$  denoting the  $\Omega$ -averaging operator. For a generic phase function  $a(\mathbf{r}, \mathbf{v}, t, \alpha)$  its configuration-space average on  $\Omega$ , can be identified respectively either with the continuous or discrete operators

$$\langle a(\mathbf{r}, \mathbf{v}, t, \alpha) \rangle_\Omega \equiv \frac{1}{\mu(\Omega)} \int_{\Omega} d^3\mathbf{r} a(\mathbf{r}, \mathbf{v}, t, \alpha) \quad (14)$$

$$\langle a(\mathbf{r}, \mathbf{v}, t, \alpha) \rangle_\Omega \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1,N} a(\mathbf{r}_i, \mathbf{v}, t, \alpha). \quad (15)$$

In practice, for actual comparisons with experimental data, both operators can be conveniently replaced by a finite summation of the form

$$\langle a(\mathbf{r}, \mathbf{v}, t, \alpha) \rangle_\Omega \cong \bar{a}^{(A)}(\mathbf{v}, t, \alpha) \equiv \frac{1}{N_*} \sum_{i=1,N_*} a(\mathbf{r}_i, \mathbf{v}, t, \alpha), \quad (16)$$

$N_*$  denoting a suitable integer to be considered  $\gg 1$ . Thus,  $\langle f_1(t) \rangle_\Omega$  should be identified with the *1-point velocity-frequency density function* (VFDF). Namely, introducing the short-way notation  $\hat{f}_1^{(freq)}(t) \equiv \hat{f}_1^{(freq)}(\mathbf{r}_i, \mathbf{v}, t, \alpha)$ , it should result

$$\langle f_1(t) \rangle_\Omega = \hat{f}_1^{(freq)}(t). \quad (17)$$

where

$$\hat{f}_1^{(freq)}(t) \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1,N} N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z) \quad (18)$$

and  $N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z)$  is the frequency associated to the fluid velocity field  $\mathbf{V}(\mathbf{r}, t, \alpha)$  [see related discussion in Appendix B and in particular Eqs. (114)-(118)]. Hence, by

definition, from Eq.(17) it follows that it must be

$$\int_U d^3\mathbf{v} \langle f_1(t) \rangle_\Omega = \int_U d^3\mathbf{v} \hat{f}_1^{(freq)}(t) = 1. \quad (19)$$

### 1C.b - The deterministic limit of $f_1$

Regarding the search of a deterministic limit for  $f_1$ , there is manifestly only one case when this can happen and it occurs in the limiting case of the stationary solution (of INSE)  $Z_o \equiv \{\mathbf{V} = \mathbf{0}, p_1 = 0\}$  (or *null solution*), for which  $f_1 \equiv \langle f_1 \rangle_\Omega$ . In fact, in such a case  $f_1$  manifestly must coincide with a distribution, i.e.,

$$\lim_{\substack{p_1 \rightarrow 0^+ \\ |\mathbf{V}| \rightarrow 0^+}} f_1 = \delta(\mathbf{v}) \quad (20)$$

(*deterministic limit*), while also there manifestly results

$$\lim_{\substack{p_1 \rightarrow 0^+ \\ |\mathbf{V}| \rightarrow 0^+}} \hat{f}_1^{(freq)}(t) = \delta(\mathbf{v}). \quad (21)$$

Since the null solution can always in principle be reached (i.e., moving backward in time and by application of a combination of appropriate volume forces and boundary conditions acting on the fluid, both to be suitably defined), it follows that Eq.(20) might always be regarded as a *possible alternative initial condition* for  $f_1$ . In the following we intend to prove that, as an example, it can be represented as the limit function

$$\delta(\mathbf{v}) \equiv \lim_{\substack{p_1 \rightarrow 0^+ \\ |\mathbf{V}| \rightarrow 0^+}} f_M(\mathbf{v}; p_1) \quad (22)$$

of a *Gaussian PDF*

$$f_M(\mathbf{v} - \mathbf{V}; p_1) = \frac{1}{\pi^2 v_{th,p}^3} \exp \left\{ -\frac{\|\mathbf{v} - \mathbf{V}\|^2}{v_{th,p}^2} \right\}, \quad (23)$$

where  $\mathbf{V} = \mathbf{0}$  and  $v_{th,p} = (2p_1/\rho_o)^{1/2}$  is the thermal velocity due to  $p_1$  [see Eq.(27)]. It is obvious, however, that the previous requirement does not provide a unique functional form for  $f_1$ . For instance, when both  $\mathbf{V}(\mathbf{r}, t, \alpha)$  and  $p_1(\mathbf{r}, t, \alpha)$  are considered infinitesimals (of order  $\varepsilon$ ), Eq.(20) only requires that

$$f_1(t) = f_M(\mathbf{u}; p_1, \alpha) + \delta f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z), \quad (24)$$

with  $\delta f_1$  infinitesimal of order  $O(\varepsilon)$ .

In the following  $\{f_1, \Gamma\}$  will be denoted as *statistically complete* if the PDF  $f_1$ :

A) admits for all  $(\mathbf{r}, t) \in \bar{\Omega} \times I$  (including the initial time  $t_o$ ) and  $G = 1, \mathbf{v}, \mathbf{u}^2/2, \mathbf{u}\mathbf{u}, \mathbf{u}\mathbf{u}^2/2$  the velocity and

phase-space moments  $\int_U d\mathbf{v} G f_1$  and  $\int_\Gamma d\mathbf{v} f_1 \ln f_1$  and satisfies the constraint equations

$$\int_U d\mathbf{v} G f_1 = 1, \mathbf{V}(\mathbf{r}, t, \alpha), p_1(\mathbf{r}, t, \alpha), \quad (25)$$

$$S(f_1(t)) = S_T. \quad (26)$$

Here  $p_1(\mathbf{r}, t, \alpha) > 0$  denotes the *kinetic pressure*

$$p_1(\mathbf{r}, t, \alpha) = p(\mathbf{r}, t, \alpha) + p_0(t, \alpha) - \phi(\mathbf{r}, t, \alpha), \quad (27)$$

with  $p_0(t, \alpha) > 0$  (the *pseudo-pressure*) a strictly positive, smooth, real function and  $\phi(\mathbf{r}, t, \alpha)$  a suitably defined potential;

B) at the initial time  $t = t_o$  satisfies the constraint (17);

C) satisfies the constraint defined by the deterministic limit (20).

The constraint equations (25)-(27), (17) and (20) are here denoted as *physical realizability conditions*.

### 1D - Open issues

Here we shall consider a class of statistical models  $\{f_1, \Gamma\}$ , based on the 1-point PDF,  $f_1$  [with  $f_1$  defined on  $\Gamma$  and  $\Gamma$  identified with (3)], which yield a *complete inverse kinetic theory for the INSE problem*. In other words, each  $\{f_1, \Gamma\}$  should yield the *complete set of fluid fields*,  $\{Z\}$ , to be represented in terms of suitable velocity moments of the same PDF. In addition,  $\{f_1, \Gamma\}$  will be required to hold for arbitrary fluid fields  $\{Z\}$  which, in the domain of existence  $\bar{\Omega} \times I$ , are strong solutions of the INSE problem, the latter - for greater generality - to be considered either *deterministic or stochastic* (see Appendix A).

In the construction of statistical models of this type several interesting issues arise, which are related both to the prescription of the initial conditions on the PDF and to its time evolution. In particular, they concern whether there exists a statistical model  $\{f_1, \Gamma\}$ , such that:

1. (*Problem 1: uniqueness condition*) both  $\{f_1, \Gamma\}$  and the PDF  $f_1$  are *unique*;
2. (*Problem 2: conditions of statistical completeness*)  $\{f_1, \Gamma\}$  is statistically complete, namely  $f_1$  satisfies the requirements posed in Subsection 1C.

Here we shall consider, in particular, the case in which the frequency  $\hat{f}_1^{(freq)}(t_o)$  is an ordinary function (i.e., not a distribution), consistent with the requirement that  $f_1$  is an ordinary function too. The second requirement is that in the limit in which  $p_1 \rightarrow 0^+$  and  $|\mathbf{V}| \rightarrow 0^+$ , there results (20).

3. (*Problem 3: moment-closure condition*) can be defined in such a way that it satisfies a *moment-closure condition*. In other words: whether there exists a finite set of moment equations of IKE (9) which are closed. This is actually a basic requirement of IKT. Hence, it should be satisfied by construction, if  $\{f_1, \Gamma\}$  relies on IKT [12].
4. (*Problem 4: kinetic-closure condition*) it can be defined in such a way that at any time  $t \geq t_o$  (with  $t \in I$ ), the statistical equation advancing in time  $f_1$  depends, besides  $f_1$ , only on a finite number of moments of the same PDF, which include necessarily the complete set of fluid fields  $\{Z(\mathbf{r}, t)\}$ . In such a case  $\{f_1, \Gamma\}$  is said to satisfy a *kinetic closure condition*. This assumption is - in some sense - analogous to the closure problem for the ML hierarchy. In both cases it effectively involves the construction of the mean-field force which advances in time the 1-point PDF.
5. (*Problem 5: determination of multi-point PDF's*) the statistical model  $\{f_1, \Gamma\}$  can be constructed in such a way that determines uniquely the multi-point PDF's, as well as the related observables.
6. (*Problem 6: closure condition of the statistical equations for multi-point PDF's*) the statistical equations for the multi-point PDF's depend only on  $f_1$ .

In the remainder a statistical model which satisfies both the moment and kinetic closure conditions indicated above in Problems 3 and 4 will be denoted as *closed*.

### 1E - Goals and scheme of presentation

Here we claim that the IKT statistical model can be defined in such a way to provide an explicit solution of problems 1-6. The construction of the 1-point PDF is achieved adopting the so-called inverse kinetic theory (IKT) for fluid dynamics (Tessarotto *et al.*, 2004-2009 [11, 12, 13, 14, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32]). This type of approach can be formulated both when the fluid is considered *regular* and *turbulent*, *i.e.* the corresponding fluid equations (INSE) and the fluid fields  $\{Z\}$  are respectively considered *deterministic* and *stochastic* [13, 14]. In particular,  $f_1$  is defined in such a way that:

A) both the PDF and the related mean-field force ( $\mathbf{F}$ ) which determines its time evolution [see Eq.(8)] are *conditional observables*. This concept [see Appendix A, Subsection A.1] is shown to imply the uniqueness and closure properties of the statistical model;

B) the PDF satisfies suitable physical realizability conditions. This requires, in particular, that the complete set of fluid fields  $\{Z\}$  is necessarily represented in terms

of moments the PDF [11, 12, 13], while the initial PDF must be defined so that its configuration-space average is suitably prescribed [see Eq.(17)]. In such a case, the solution of the initial condition for  $f_1$  (see Problem 2) is uniquely achieved by invoking the Principle of Entropy Maximization (PEM; Jaynes, 1957 [33]). This permits to identify two possible solutions for the initial PDF, corresponding respectively to the initial condition  $1_A$  and to  $1_B$  jointly.

The first one is realized by a local Gaussian PDF ( $f_M$ ).

The formulation of the corresponding statistical model  $\{f_M, \Gamma\}$  and the analysis of its basic properties are discussed in Section 2. First, it is pointed out that PEM requires necessarily that  $f_1 \equiv f_M$  must be a conditional observable for all  $t \in I$ . Then, by identifying the mean-field force  $\mathbf{F}(f_M)$  with a conditional observable, it is proven that it is uniquely defined, both as a function of the kinetic velocity  $\mathbf{v}$  (actually a polynomial of second degree with respect the relative kinetic velocity  $\mathbf{u} = \mathbf{v} - \mathbf{V}$ ) and of the fluid fields  $\{Z\} \equiv \{\mathbf{V}, p_1\}$ . As a consequence, the statistical model  $\{f_M, \Gamma\}$  is unique (THM.1; see also Problem 1). Moreover, the complete set of fluid fields  $\{Z\}$  are uniquely determined as moments of  $f_M$ , which means that the classical dynamical system defined by the initial-value problem (7) determines uniquely both the time-evolution of the PDF and of the complete set of fluid fields  $\{Z\}$ . However, unless the initial constraint (17) is fulfilled by  $f_M$  (which is generally not the case),  $\{f_M, \Gamma\}$  is not statistically complete (see Corollary to THM.1).

The construction of the statistical model  $\{f_1, \Gamma\}$  which takes into account such a case is carried out in Section 3. The condition of statistical completeness requires that the initial PDF satisfied simultaneously conditions  $1_A$  and  $1_B$ . It is found that this generally provides (at  $t = t_o$ ) a non-Gaussian initial PDF of prescribed form (see THM.2). Its time evolution depends now on the mean-field force  $\mathbf{F}(f_1)$ . Under the assumptions that its dependence in terms of the kinetic velocity  $\mathbf{v}$  can only occur, as in the Gaussian PDF, only via a polynomial of second degree in  $\mathbf{u}$  and identifying  $\mathbf{F}(f_1)$ , as in the previous case, with a conditional observable its form is found to be unique as the statistical model  $\{f_1, \Gamma\}$  while  $\{f_1, \Gamma\}$  is also statistically complete.

In the same section (Subsection 3D) the closure problem (Problems 3 and 4), based on the IKT statistical model, is formulated. This refers, in particular, to the construction of its formal solution (*i.e.*, see also paragraphs 1B and 1D). This is achieved, *both for deterministic and stochastic fluids described by the INSE problem* (as defined in Appendix A). In our theory this is done by determining directly  $f_1$ , rather than its stochastic average  $\langle f_1 \rangle$ . As a basic consequence, it follows that the statistical equation for  $f_1$  is necessarily closed, namely it depends only on  $f_1$  and a finite number of moments of the same PDF. The proof of the closure property of the IKT statistical model is proven in THM.3.

There are several new contributions and basic consequences of the theory here presented.

Besides the (generally non-Gaussian) characterization of the initial PDF, it is found that, both for regular and turbulent flows, its time evolution is provided by a Liouville equation, while the corresponding Liouville operator depends only on a finite number of velocity moments of the same PDF. Hence, its time evolution depends (functionally) solely on the same (1-point) PDF. An interesting issue is also provided by the comparison, carried out in section 4, between  $\{f_1, \Gamma\}$  and the common statistical model, denoted  $\{f_H, \Gamma\}$ , laying at the core of the customary statistical approaches [i.e., the HRE [1, 2, 3] and ML [7, 8] approaches]. The latter, although both unique and closed (in the sense of Problems 3 and 4), is proven to be *statistically incomplete* (see THM.4), since the corresponding PDF cannot generally fulfill the physical constraint placed on it by Eq.(17) [at  $t = t_o$  or at any time  $t \in I$ ].

The connection with previous statistical approaches is investigated. In particular, it is shown that  $f_1$  can be identified with a suitable stochastic average of the PDF  $f_H$  (see THM.5). A remarkable consequence of the present theory is that it affords the *exact construction* of the corresponding statistical equation for the stochastic-averaged PDF.(Section 4). The latter is shown to depart from the customary transport equation considered in the literature [see, for example, Dopazo [5] and Pope [6]]. The relationship with the Hopf functional-differential method [1] is also displayed.

Finally, the explicit construction of multi-point PDF's and of the related observables (Section 5) is achieved. In particular, the statistical evolution equations for the multi-point PFD's are shown to maintain the form of Liouville equations. As a practical application, the explicit construction of reduced 2-point PDF's - and of their related statistical equations - both usually investigated in experimental/numerical research in fluid dynamics, is presented. In fact, despite not being themselves observables, they are nevertheless related to physical observables (or conditional observables), such as the velocity difference between different fluid elements, usually adopted for the statistical analysis of turbulent fluids. Finally, in Section 6 the conclusions are drawn.

## 2 - IKT APPROACHES

A fundamental aspect of fluid dynamics is the construction of statistical models  $\{f_1, \Gamma\}$  in which the 1-point PDF is the solution of a so-called *inverse problem*, involving the search of a so-called inverse kinetic theory (IKT) able to yield the complete set of fluid equations for the fluid fields. A particular realization for  $\{f_1, \Gamma\}$  is provided by (the already mentioned) ML approach,

which is based on the position (11) and the particular solution (12). In such a case it follows, by construction, that  $f_1$  depends explicitly, and not just merely in a functional sense, on the fluid field  $\mathbf{V}(\mathbf{r}, t)$ . Hence, IKE (9) implies necessarily INSE (and therefore can be viewed as an inverse kinetic equation). Nevertheless, it is obvious that the fluid pressure  $p(\mathbf{r}, t)$  *cannot be represented as a moment of the same PDF*.

In this connection, however, a more general viewpoint is represented by the search of so-called *complete IKT's* able to yield as moments of the PDF the *whole set of fluid fields*  $\{Z\}$  which determine the fluid state and in which the same PDF satisfies a Liouville equation. This implies that in such a case *there must exist a classical dynamical system, of the type defined by Eq.(6), whose evolution operator  $T_{t_o, t}$  advances in time both the PDF and the related fluid fields, while preserving - at the same time - a suitable probability measure* (Frisch, 1995 [19]). Despite previous attempts (Vishik and Fursikov, 1988 [20] and Ruelle, 1989 [21]) the existence of such a dynamical system has remained for a long time an unsolved problem.

This type of approach has actually been achieved for incompressible NS fluids [11, 12], with the discovery of the (corresponding) *NS dynamical system* which advances in time the complete set of fluid fields  $\{Z\}$ . Its applications and extensions are wide-ranging and concern in particular: incompressible thermofluids [25], quantum hydrodynamic equations (see [23, 26]), phase-space Lagrangian dynamics [27], tracer-particle dynamics for thermofluids [28, 32], the evolution of the fluid pressure in incompressible fluids [29], turbulence theory in Navier-Stokes fluids [13, 25] and magnetofluids [14] and applications of IKT to lattice-Boltzmann methods [31]. In the following we intend to investigate, in particular, its consequences for the problems posed in this paper.

### 2A - The IKT statistical model - Basic assumptions

Let us now show how a statistical model of this type for the 1-point PDF [i.e.,  $\{f_1, \Gamma\}$ ], which fulfills the requirements posed in Problems 1-5 and holds both for regular and stochastic flows [13, 14], can be achieved by suitably modifying the IKT approach earlier developed by Tessarotto and coworkers [11, 12] (see also Ref.[13]).

Such a theory, it must be stressed, is based on some of the axioms (such as the conservation of entropy, the principle of entropy maximization or the regularity assumptions) which are typical of CSM. In particular, the IKT of Refs. [12, 23]) requires that  $f_1(t) \equiv f_1(\mathbf{x}, t, \alpha; Z)$  is a particular solution of the 1-point IKE (9) and satisfies the following assumptions (Axioms #0-#4), imposing that for all  $(\mathbf{x}, t) \in \bar{\Gamma} \times I$ :

- (Axiom #0: regularity)  $f_1(t)$  is an ordinary,

strictly positive function. By assumption it is measurable, i.e., it admits the velocity- and phase-space moments

$$\int_U d\mathbf{v} G f_1 \quad (28)$$

respectively for  $G = 1, \mathbf{v}, \rho_o u^2/3, \mathbf{u}\mathbf{u}, \mathbf{u}\mathbf{u}^2/3$  and for  $S(f_1(t)) = - \int_{\Gamma} d\mathbf{x} f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z) \ln f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z)$ , the so-called Boltzmann-Shannon (BS) entropy. Moreover,  $f_1$  is suitably smooth, in the sense that it is continuous  $\overline{\Gamma} \times I$ , is a particular solution of IKE (9) and its velocity moments  $G_2, G_3 \equiv \mathbf{v}, \rho_o u^2/3$  are respectively of class

$$\begin{cases} G_2 \in C^{(3,1)}(\Omega \times I), \\ G_3 \in C^{(2,0)}(\Omega \times I); \end{cases} \quad (29)$$

- (*Axiom #1: principle of correspondence*)  $f_1(t)$  satisfies identically in  $\overline{\Omega} \times I$  the constraints (25)-(27) and the fluid fields (including the kinetic pressure  $p_1$ ) can be considered (conditional) observables. As a part of the same axiom it is required, furthermore, that  $f_1(\mathbf{r}, \mathbf{u}, t; Z)$  satisfies suitable kinetic initial and boundary conditions [see Ref.]. The latter are defined so that, by construction, the moments (25)-(27) identically satisfy the initial and boundary conditions prescribed by the INSE problem [see Eqs.(92) and (93) in Appendix A];
- (*Axiom #2: moment-closure condition*) the moments equations, corresponding to  $G = 1, \mathbf{v}, \rho_o u^2/3$  and evaluated in terms of IKE (9), define a system of closed equations, which coincide with the complete set of fluid equations provided by INSE [see Eqs.(88)-(90) in Appendix A];
- (*Axiom #3: principle of conservation of entropy, or constant H-theorem*)  $f_1(t)$  satisfies the constraint equation [also known as constant H-theorem [23]]

$$\frac{\partial}{\partial t} S(f_1(t)) = 0. \quad (30)$$

- (*Axiom #4: maximum entropy principle*)  $f_1(t)$  satisfies, at  $t = t_o$ , the *constrained maximal variational principle* (also known as principle of entropy maximization or PEM; Jaynes, 1957 [33]):

$$\delta S(f_1(t)) = 0. \quad (31)$$

In this paper we shall impose, furthermore, two new assumptions introduced to satisfy the previous problems (*Problem 1-7*), requiring that:

- (*Assumption #1: conditional observables*)  $f_1$  and the mean-field force  $\mathbf{F}$  are *conditional observables*;
- (*Assumption #2: statistical completeness*)  $\{f_1, \Gamma\}$  is statistically complete, namely  $f_1$ , satisfies the *physical realizability conditions* placed by: (Assumption #2a) the velocity moments (25)-(27); (Assumption #2b) the VFDF, i.e., Eq.(17); (Assumption #2c) the deterministic limit (20).

*In the remainder Axioms #0-4 will be assumed to hold, together with Assumption #1 and #2, for the statistical model  $\{f_1, \Gamma\}$ .*

## 2B - The Gaussian particular solution

Let us now show that imposing PEM (at  $t = t_o$ ) and requiring solely the specification of its functional class  $\{f_1\}$  - i.e., not imposing also the validity of the initial constraint equation (17) for the 1-point PDF - uniquely determines its initial value  $f_1(t_o) \equiv f(\mathbf{x}, t_o, \alpha; Z)$ .

For definiteness, let us assume that  $f_1(t_o)$  is an ordinary, strictly positive function, requiring initially that it *satisfies only the constraint provided by the fluid fields*, namely Eq.(92) [Assumption #2a] and by the deterministic limit (20) [Assumption #2c]. Invoking the method of Lagrange multipliers, the PEM variational principle [(31)] implies that at the initial time  $t_o$  and for arbitrary variations  $\delta f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z)$  it must result identically:

$$\int_{\Gamma} d\mathbf{x} \delta f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z) \{ 1 + \ln f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z) + \lambda_o + \lambda_1 \cdot \mathbf{u} + \lambda_2 \mathbf{u}^2 \} = 0. \quad (32)$$

Here  $\lambda_o, \lambda_1$  and  $\lambda_2$  are Lagrange multipliers to be determined by imposing the correspondence principle [i.e., the moment equations (25)]. It follows that: 1) at  $t = t_o$ ,  $f_1(\mathbf{r}, \mathbf{u}, t_o, \alpha; Z)$  necessarily coincides with a Gaussian distribution (23) [12, 23] carrying the fluid velocity  $\mathbf{V}(\mathbf{r}, t_o, \alpha)$  and the kinetic pressure  $p_1(\mathbf{r}, t_o, \alpha)$ ; 2) Axiom #0 implies that  $p_1(\mathbf{r}, t_o)$  must be strictly positive; 3)  $f_M(t_o)$  is necessarily a conditional observable, so that when  $\alpha$  and  $\mathbf{v}$  (or the relative kinetic velocity  $\mathbf{u}$ ) are considered prescribed,  $f_M(\mathbf{u} \equiv \mathbf{v} - \mathbf{V}(\mathbf{r}, t_o, \alpha); p_1(\mathbf{r}, t_o, \alpha))$  is unique and depends in a prescribed way only on observables; 4) moreover, due to the arbitrariness of the choice of the initial time  $t_o$ , the Gaussian PDF (23) is necessarily a particular solution of IKE (9) for all  $t \in I$ ; 5) as a consequence, also the same equation at all times is a conditional observable in the sense indicated above.

On the other hand, imposing for Eq.(9) the particular solution

$$f_1(\mathbf{r}, \mathbf{u}, t, \alpha; Z) \equiv f_M(\mathbf{u}; p_1(\mathbf{r}, t, \alpha)) \quad (33)$$

implies that the vector field  $\mathbf{F}$  must depend functionally on  $f_M$  and  $\{Z\}$ , i.e., it is of the type  $\mathbf{F}(f_M) \equiv \mathbf{F}(\mathbf{x}, t; f_M)$

[12, 23]. One finds, however, that the most general *admissible form* of the vector field  $\mathbf{F}(f_M)$  [namely one which is consistent with the requirement (33)], is of the type:

$$\begin{aligned}\mathbf{F}(\mathbf{x}, t, \alpha; f_M) = & \mathbf{F}_0(\mathbf{x}, t, \alpha; f_M) + \\ & + \mathbf{F}_1(\mathbf{x}, t, \alpha; f_M) + \Delta\mathbf{F}(\mathbf{x}, t, \alpha; f_M).\end{aligned}\quad (34)$$

Here  $\Delta\mathbf{F}$  is an arbitrary "gauge" vector field satisfying the homogeneous equation

$$\frac{\partial}{\partial \mathbf{v}} \cdot (\Delta\mathbf{F} f_M) = 0, \quad (35)$$

i.e., it does not contribute to IKE when Eq.(33) holds identically, while  $\mathbf{F}_0$ ,  $\mathbf{F}_1$  and  $A(\mathbf{r}, t; f_M)$  are respectively the vector and scalar fields

$$\begin{aligned}\mathbf{F}_0(\mathbf{x}, t, \alpha; f_M) = & \frac{1}{\rho_0} \mathbf{f}_R + \\ & + \frac{1}{2} \mathbf{u} \cdot \nabla \mathbf{V} + \frac{1}{2} \nabla \mathbf{V} \cdot \mathbf{u} + \nu \nabla^2 \mathbf{V},\end{aligned}\quad (36)$$

$$\begin{aligned}\mathbf{F}_1(\mathbf{x}, t, \alpha; f_M) = & \frac{1}{2} \mathbf{u} A(\mathbf{r}, t; f_M) + \\ & + \frac{v_{th}^2}{2} \nabla \ln p_1 \left\{ \frac{u^2}{v_{th}^2} - \frac{3}{2} \right\},\end{aligned}\quad (37)$$

$$\begin{aligned}A(\mathbf{r}, t, \alpha; f_M) \equiv & \frac{1}{p_1} \frac{\partial}{\partial t} p_1 - \frac{\rho_o}{p_1} \left[ \frac{\partial}{\partial t} V^2 / 2 + \right. \\ & \left. + \mathbf{V} \cdot \nabla V^2 / 2 - \frac{1}{\rho_o} \mathbf{V} \cdot \mathbf{f} - \nu \mathbf{V} \cdot \nabla^2 \mathbf{V} \right].\end{aligned}\quad (38)$$

Then, by construction  $\mathbf{F}_0$  and  $\mathbf{F}_1$  are conditional observables. In particular Eq.(35) requires

$$\Delta\mathbf{F}(\mathbf{x}, t, \alpha; f_M) = \mathbf{u} \cdot \underline{\underline{\mathbf{E}}} \equiv \Delta\mathbf{F}_1(\mathbf{x}, t, \alpha; f_M), \quad (39)$$

where  $\underline{\underline{\mathbf{E}}} \equiv \underline{\underline{\mathbf{E}}}(\mathbf{r}, t)$  is an arbitrary antisymmetric second-order tensor. From Eq.(39) it follows that  $\Delta\mathbf{F}$  is manifestly non-observable. In fact, introducing the transformation

$$\Delta\mathbf{F} \rightarrow \Delta\mathbf{F}' = k \Delta\mathbf{F} \quad (40)$$

with  $k \in \mathbb{R}$  arbitrary and non-vanishing, it yields for  $\mathbf{F}$  an admissible form too [i.e., consistent with Eq.(33)].

## 2C - Properties of $\{f_M, \Gamma\}$

Let us now pose the problem of resolving the indeterminacy of  $\mathbf{F}(f_M)$ . In Refs. [23, 24] for Gaussian solutions the uniqueness of  $\mathbf{F}$  was achieved based on the requirement of consistency with extended thermodynamics, namely by imposing a suitably-prescribed form for

higher-order moments of the Liouville equation. In particular this was found to require

$$\Delta\mathbf{F} \equiv \mathbf{0}. \quad (41)$$

Here we point out, however, that Eq.(41) is equivalent to impose that  $\mathbf{F}(\mathbf{x}, t, \alpha; f_M)$  is a *conditional observable* (see Assumption #2), namely a uniquely-prescribed (polynomial) function of the kinetic velocity  $\mathbf{v}$  (as well of the variables and  $\mathbf{r}, t, \alpha$ ). Hence, the following theorem holds:

### THM.1 - Uniqueness of $\{f_M, \Gamma\}$

*In validity of Assumptions #1, 2 and 3a, 3c the statistical model  $\{f_M, \Gamma\}$  defined by Eqs.(23), with mean-field force  $\mathbf{F}(\mathbf{x}, t, \alpha; f_M)$  prescribed by Eqs.(34)-(38) and subject to the constraint (41), is unique.*

#### PROOF

The proof is immediate. Uniqueness follows, in fact, besides the axioms of IKT (Axioms #0-4), from the requirement that both  $f_M$  and  $\mathbf{F}(\mathbf{x}, t, \alpha; f_M)$  be conditional observables and hence, in particular, from Eq.(41). Q.E.D.

In Ref. [12] the statistical model  $\{f_M, \Gamma\}$  was proven to determine uniquely, thanks to Axiom #1, the complete set of fluid fields. Such a result holds, however, in principle for an arbitrary choice of  $\Delta\mathbf{F}$  of the form (39), namely also in the case in which  $\Delta\mathbf{F} \neq \mathbf{0}$ . In Refs. [23, 24] the uniqueness of the mean-field force for the Gaussian PDF ( $f_M$ ) was achieved based on phenomenological arguments, i.e., the comparison with extended thermodynamics. The present result shows, however, that uniqueness for  $\mathbf{F}(\mathbf{x}, t, \alpha; f_M)$ , and hence  $\{f_M, \Gamma\}$  too, can actually be achieved based on the physical prescription that both quantities are conditional observables (see Assumptions #1 and 2).

Nevertheless, it is obvious that the statistical model  $\{f_M, \Gamma\}$  generally is *not statistically complete*, in the sense indicated above. In fact (generally)  $f_M$  does not satisfy the constraint imposed by the initial condition (17). There it follows immediately:

### COROLLARY to THM.1 - Statistical incompleteness of $\{f_M, \Gamma\}$

*In validity of THM.1 the statistical model  $\{f_M, \Gamma\}$  is generally statistically incomplete.*

#### PROOF

We notice that for a Gaussian PDF (23) the deterministic limit (20) exists. This requires letting  $p_1 \rightarrow 0^+$  and  $|\mathbf{V}| \rightarrow 0^+$ , implying also that  $p_1$  must be uniquely determined (i.e., it is necessarily an observable). However, it is obvious the constraint (92) may not be fulfilled by  $f_M$ . In fact, there results generally at  $t = t_o$  (for finite  $p_1$  and  $|\mathbf{V}|$ )

$$\frac{\widehat{f}_1^{(freq)}(\mathbf{v}, t, \alpha; Z)}{\langle f_M \rangle_\Omega} \neq 1. \quad (42)$$

Q.E.D.

This leaves open the question of extending IKT in such a way to satisfy this requirement (of statistical completeness). In the remainder we intend to show that this constraint generally implies a non-Gaussian initial PDF.

### 3 - IKT STATISTICAL MODEL: NON-GAUSSIAN CASE

An interesting question is posed by the case in which the PDF at  $t = t_o$ ,  $f_1(t)$  satisfies also the initial condition determined by Eq. (17) [Assumption #2b]. If the fluid velocity  $\mathbf{V}(\mathbf{r}, t)$  is bounded in the domain  $\overline{\Omega}$ , the constraint (17) implies necessarily that the subdomain of velocity space in which  $f_1$  remains strictly positive is generally a bounded subset of  $\mathbb{R}^3$ . Hence, this prescription generally corresponds to an initial 1-point PDF which is locally *non-Gaussian*, specifically because of the (missing) tails of the PDF.

#### 3A - Solution of the initial-value problem for $f_1$

In this case, let us consider (at  $t = t_o$ )  $f_1$  of the general form

$$f_1(t) = \langle f_1(t) \rangle_{\Omega} \frac{h(t)}{\langle h(t) \rangle_{\Omega}}, \quad (43)$$

with  $\langle f_1(t_o) \rangle_{\Omega}$  determined by Eq.(17) and  $h(t_o)$  to be assumed again as a strictly positive and regular real function. Then considering variations of  $f_1$  the type

$$\delta f_1 = \langle f_1 \rangle_{\Omega} \frac{\delta h}{\langle h \rangle_{\Omega}}, \quad (44)$$

i.e., defined so that there results identically  $\delta \langle f_1 \rangle_{\Omega} = \delta \langle h \rangle_{\Omega} \equiv 0$ , the variational principle (31) (PEM) requires in this case that at the initial time  $t_o$ ,  $h(t_o)$  must fulfill the variational equation

$$\int_{\Gamma} d\mathbf{x} \delta h(t_o) \frac{\langle f_1 \rangle_{\Omega}}{\langle h \rangle_{\Omega}} \{ 1 + \ln h(t_o) + \lambda_o + \lambda_1 \cdot \mathbf{u} + \lambda_2 \mathbf{u}^2 \} = 0. \quad (45)$$

Thus,  $f_1(t_o)$  is necessarily of the form (43), while at  $t = t_o$  the function  $h(t)$  reads

$$h(t) = \exp \{ -1 - \lambda_o - \lambda_1 \cdot \mathbf{u} - \lambda_2 \mathbf{u}^2 \}, \quad (46)$$

with the Lagrange multipliers  $\lambda_o, \lambda_1$  and  $\lambda_2$  to be determined again imposing the moment equations (25). It follows that:

1. due to the arbitrariness of the choice of  $t_o$ , thanks to Axioms #3 (conservation of the BS entropy) and 4 (PEM), it follows that for all  $t \in I$ ,  $f_1(t)$  is necessarily of the form (43);

2. unless there results identically  $\frac{\langle f_1 \rangle_{\Omega}}{\langle h \rangle_{\Omega}} = 1$ , the initial PDF  $f_1(t_o)$  is *generally not a Gaussian*, and hence of the form  $f_1(t) = g_1(t)f_M(t)$ , with  $g_1(t) \neq 1$  to be assumed a suitably smooth ordinary function;
3.  $f_1(t_o)$  is necessarily a conditional observable (Assumption #1).

#### 3B - The Liouville evolution equation for $f_1$

To determine the time evolution of the PDF we require again that the mean field force  $\mathbf{F}(f_1) \equiv \mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  is a conditional observable. To determine explicitly  $\mathbf{F}(f_1)$ , let us require, first, that when Eq.(33) holds identically,  $\mathbf{F}(f_1)$  must coincide with  $\mathbf{F}(f_M)$  [defined by Eqs.(34)-(39)]. The same manifestly must occur if  $f_1$  remains, in the whole phase space  $\Gamma$ , suitably "near" to  $f_M$ . In fact, in this case in the same set  $\mathbf{F}(f_1)$  and  $\mathbf{F}(f_M)$  must remain close too (again in some suitable asymptotic sense). This delivers for  $\mathbf{F}(f_1)$  a prescribed polynomial representation in terms of the relative kinetic velocity  $\mathbf{u}$ . In principle, in fact,  $\mathbf{F}(f_1)$  might include also polynomials of higher-degree in  $\mathbf{u}$ . These terms, however, must necessarily vanish identically for  $f_1 \equiv f_M$  and cannot contribute to the moment equations [of IKE] which yield INSE. Since their form remains therefore arbitrary, they are manifestly non-observables. *Hence such terms are ruled out by the requirement of  $\mathbf{F}(f_1)$  being a conditional observable.* This implies that  $\mathbf{F}(f_1)$  must be necessarily a polynomial of second degree in the relative kinetic velocity  $\mathbf{u}$ , whose precise form is prescribed by imposing that the moment equations of IKE for  $G(\mathbf{v}, \mathbf{r}, t) = 1, \mathbf{v}, \rho_o u^2 / 3$  must necessarily coincide with INSE [ Eqs.(88)-(90) in Appendix A]. Let us introduce now the mean-field force:

$$\begin{aligned} \mathbf{F}(\mathbf{x}, t, \alpha; f_1) &= \mathbf{F}_0(\mathbf{x}, t, \alpha; f_1) + \mathbf{F}_1(\mathbf{x}, t, \alpha; f_1) + (47) \\ &+ \Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1), \end{aligned} \quad (48)$$

$\Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  denoting here an arbitrary gauge vector field of the form

$$\Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1) = \Delta \mathbf{F}_1(\mathbf{x}, t, \alpha; f_M) + \Delta \mathbf{F}_2(\mathbf{x}, t, \alpha; f_1),$$

defined so that: a) if  $f_1 \equiv f_M$ , it coincides with

$$\Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1) = \Delta \mathbf{F}_1(\mathbf{x}, t, \alpha; f_M);$$

b) it does not contribute to the moment equations of IKE, evaluated for  $G(\mathbf{v}, \mathbf{r}, t) = 1, \mathbf{v}, \rho_o u^2 / 3$ , namely it is defined so that there results identically

$$\int d^3 v \Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1) f_1 = \mathbf{0}. \quad (49)$$

Hence  $\Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  satisfies manifestly the gauge condition (40). The indeterminacy of  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  can avoided

again by imposing again the requirement that it is a conditional observable (Assumption #2), namely

$$\Delta \mathbf{F}(\mathbf{x}, t, \alpha; f_1) \equiv 0. \quad (50)$$

Here the vector fields  $\mathbf{F}_0$  and  $\mathbf{F}_1$  are [12]

$$\begin{aligned} \mathbf{F}_0(\mathbf{x}, t, \alpha; f_1) &= \frac{1}{\rho_0} [\nabla \cdot \underline{\underline{\Pi}} - \nabla p_1 + \mathbf{f}_R] + \quad (51) \\ &+ \frac{1}{2} \mathbf{u} \cdot \nabla \mathbf{V} + \frac{1}{2} \nabla \mathbf{V} \cdot \mathbf{u} + \nu \nabla^2 \mathbf{V}, \end{aligned}$$

$$\begin{aligned} \mathbf{F}_1(\mathbf{x}, t, \alpha; f_1) &= \frac{1}{2} \mathbf{u} \left\{ A(\mathbf{r}, t; f) + \frac{1}{p_1} \nabla \cdot \mathbf{Q} - \right. \quad (52) \\ &\left. - \frac{1}{p_1^2} [\nabla \cdot \underline{\underline{\Pi}}] \cdot \mathbf{Q} \right\} + \frac{v_{th}^2}{2p_1} \nabla \cdot \underline{\underline{\Pi}} \left\{ \frac{u^2}{v_{th}^2} - \frac{3}{2} \right\}, \end{aligned}$$

with  $\mathbf{Q}$  and  $\underline{\underline{\Pi}}$  denoting the moments

$$\begin{cases} \mathbf{Q} = \rho_o \int d^3 v \mathbf{u} \frac{u^2}{3} f_1, \\ \underline{\underline{\Pi}} = \rho_o \int d^3 v \mathbf{u} \mathbf{u} f_1, \end{cases} \quad (53)$$

and the scalar field  $A(\mathbf{r}, t, \alpha; f_1)$  defined by Eq.(38).

### 3C - Properties of $\{f_1, \Gamma\}$

Let us now prove that the IKT statistical model  $\{f_1, \Gamma\}$  satisfies both Problems #1 and 2 also for non-Gaussian PDF's of the type (43). As a consequence, the following theorem holds:

#### THM.2 - Uniqueness and statistical completeness of $\{f_1, \Gamma\}$

*In validity of Assumptions #1, 2 and 3 (i.e., 3a-3c), let us impose that the statistical model  $\{f_1, \Gamma\}$  is defined by requiring that  $f_1$  is a strictly positive ordinary function which satisfies the initial condition (43) with (46) and IKE (9), with the corresponding mean field force defined by Eqs.(47)-(52). Then  $\{f_1, \Gamma\}$  is unique and statistically complete.*

#### PROOF

In fact, first, the initial condition (43) determined imposing PEM together with the constraints (92) and (17) is manifestly unique and hence a  $f_1(t_o)$  is necessarily conditional observable. Furthermore, thanks to Assumption #2  $\mathbf{F}(\mathbf{x}, t; f_1)$  is necessarily of the form provided by Eqs. (47)-(52), i.e., unique, so that  $\{f_1, \Gamma\}$  is unique too. Second, the initial PDF satisfies by construction also to the requirement posed by Eq.(17). Let us now prove that  $f_1$  fulfills also the deterministic limit (20). This follows invoking Eq.(21) and noting that in the limit  $p_1 \rightarrow 0^+$  and  $|\mathbf{V}| \rightarrow 0^+$  there results manifestly

$$\lim_{\substack{p_1 \rightarrow 0^+ \\ |\mathbf{V}| \rightarrow 0^+}} \frac{h(t)}{\langle h(t) \rangle_\Omega} = 1. \quad (54)$$

This proves that  $\{f_1, \Gamma\}$  is statistically complete too. Q.E.D.

We remark that:

- the proof that  $\{f_1, \Gamma\}$  provides a complete IKT for the INSE problem was reached previously in Ref. [12]. This follows by noting that, by construction, (thanks to Axioms #0-2) the fluid fields  $\{\mathbf{V}, p_1\}$  necessarily satisfy the INSE initial-boundary value problem [see Appendix A], when they are identified with the two velocity moments of the PDF evaluated for  $G = \mathbf{v}, \rho_o u^2/3$ .
- THM.2 yields a solution to Problem #1, namely that the initial the 1-point PDF coincides with the observable defined by the initial VDFD  $\widehat{f}_1^{(freq)}(\mathbf{v}_j, t_o, \alpha; Z)$  [see Eq.(17)];
- In particular, THM.2 (as also THM.1) holds *both in the case in which the fluid fields are deterministic and stochastic, i.e., both for the deterministic and stochastic INSE problems* [defined in Appendix A];
- In case of THM.2 the assumption that both the 1-point PDF  $f_1$  and  $\mathbf{F}$  are conditional observables (Assumptions #1 and 2) is ultimately demanded also by consistency with the physical requirement posed by the constraint (17). In fact, it is obvious that otherwise the uniqueness of  $\{f_1, \Gamma\}$  might not be warranted. In particular, this means that configuration-space average of the PDF, i.e., either the continuous or discrete averages  $\langle f_1 \rangle_\Omega$  and  $\overline{f}_1$  might not be unique, and hence these quantities *would not be observables*;
- In Refs. [23, 24] the uniqueness of the mean-field force  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  for a non-Gaussian  $f_1$ , was achieved again based both on phenomenological arguments, i.e., besides the comparison with extended thermodynamics, the requirement that  $\mathbf{F}$  depends only on the minimum number of higher-order moments of  $f_1$ , defined so that: a) they provide the correct fluid equations; b) they vanish identically in the case (33). THM.2 shows that the uniqueness [of  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$ ] is achieved simply based on the physical prescription that both  $f_1$  and  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  are conditional observables (see again Assumptions #1 and 2).

### 3D - Solution of the closure problem

As indicated above, a desired property of statistical models in fluid dynamics would be the (possible) fulfillment of suitable closure conditions, permitting to assure that the relevant PDF advances in time by means of a statistical equation which depends solely on the same PDF.

Here we wish to investigate the closure problem earlier posed [Subsections 1B and 1D] and, in particular, that specified by Problems 4 and 5. It is immediate to prove that a *formal exact solution* for such closure problems is provided by the IKT statistical model  $\{f_1, \Gamma\}$  defined in the previous sections 2 and 3. In other words,  $\{f_1, \Gamma\}$  is necessarily closed, i.e., the following result holds:

### THM.3 - Closure properties of $\{f_1, \Gamma\}$ (Closure Theorem)

*In validity of Assumptions #1, 2 and 3 (i.e., 3a-3c), the statistical model  $\{f_1, \Gamma\}$ , defined by imposing the initial condition (43) with (46), and with  $f_1(\mathbf{r}, \mathbf{v}, t)$  assumed as a strictly positive ordinary function satisfying IKE (9), with mean field force defined by Eqs.(47)-(52), is closed.*

PROOF

Due to the prescription (34)-(38) of the mean-field force  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  it is immediate to prove that the moment equations of IKE for  $G = 1, \mathbf{v}, \rho_o u^2/3$ , namely

$$\int_U d^3 \mathbf{v} G L f_1 = 0 \quad (55)$$

coincide respectively with Eq.(89) (for the moments  $G = 1$  and  $\rho_o u^2/3$ ) and with Eq.(90) (for the second moment  $G = \mathbf{v}$ ), i.e., with the complete set of PDE defined by INSE [see Eqs. (88)- 93, in Appendix A]. The latter, by assumption, define a closed system of equations, hence the moment-closure condition (Problem 4) is necessarily satisfied. Furthermore, to prove that also the kinetic-closure condition (posed by Problem 5) holds it is sufficient to notice that the same mean-field force  $\mathbf{F}(\mathbf{x}, t, \alpha; f_1)$  depends, by construction, only on the fluid fields  $\mathbf{V}, p_1, \mathbf{Q}$ , and  $\underline{\Pi}$ . Therefore, also the requirement of kinetic-closure is necessarily satisfied. Q.E.D.

### 4 - COMPARISONS WITH PREVIOUS APPROACHES

Interesting issues are posed by the comparison with previous statistical treatments and in particular the statistical model  $\{f_H, \Gamma\}$ , underlying both the HRE [1, 2, 3] and ML [7, 8] approaches. This is relevant in special reference to:

- analyze basic properties of  $\{f_H, \Gamma\}$  (see Subsection 4A);
- determine the explicit relationship between the PDF's  $f_1$  and  $f_H$ , which characterize the two approaches (Subsection 4B);
- the construction of the statistical equation for the stochastic-average of  $f_1$  (Subsection 4C),
- the comparison with the HRE functional-differential approach (Subsection 4D).

### 4A - Properties of $\{f_H, \Gamma\}$

It is immediate to show that  $\{f_H, \Gamma\}$ : 1) holds both for the deterministic and stochastic INSE problems [see Appendix A]; 2) realizes an IKT for INSE, which is *unique* and *closed*; 3) it is (generally) not a *complete IKT* (in fact, manifestly, neither the fluid pressure, nor the kinetic pressure, can be represented in terms of velocity moments of  $f_H$ ); 4) in addition, it is (generally) *not statistically complete*. Indeed, since  $f_H$  is a distribution, its configuration-space average cannot generally expected to agree with the observable  $\widehat{f}_1^{(freq)}(\mathbf{v}, t, \alpha; Z)$  or VDFD (1-point velocity-frequency density function). The following result holds:

### THM.4 - Statistical incompleteness of $\{f_H, \Gamma\}$

*The statistical model  $\{f_H, \Gamma\}$  does not generally fulfill the constraint (17).*

PROOF

To reach the proof, let us evaluate the configuration-space average of  $f_H$ . For definiteness, let us adopt the definition of discrete average provided by Eq.(16). Thus, by denoting  $Z_i \equiv \{\mathbf{V}_i(t), p_i(t)\}$  the average fluid fields in the  $i$ -th cell of  $\Omega$  (and evaluated at position  $\mathbf{r}_i$ ), it follows that the configuration-space average of  $f_H$  reads

$$\langle f_H(t) \rangle_\Omega = \frac{1}{N_*} \sum_{i=1, N_*} \delta(\mathbf{v} - \mathbf{V}_i(t)), \quad (56)$$

i.e.,  $\langle f_H \rangle_\Omega(\mathbf{v}, t)$  is still a distribution. Hence, it cannot generally be identified with the observable  $\widehat{f}_1^{(freq)}$  (which by assumption here it is considered as an ordinary function)! For comparison, instead, the complete IKT approach yields instead:

$$\langle f_1(t) \rangle_\Omega = \frac{1}{N_*} \sum_{i=1, N_*} f_1(t). \quad (57)$$

where in this case by definition  $f_1$  is an ordinary function (and hence its configuration-space average  $\langle f_1(t) \rangle_\Omega$  can be identified with the observable/conditional observable  $\widehat{f}_1^{(freq)}(t)$ , which - on the contrary is generally an ordinary function. Q.E.D.

A similar proof can be achieved also adopting the continuous operator (14). We remark here that:

1. the setting based on the definition (16) is actually consistent with the physical measurement process of the corresponding 1-point velocity frequency  $[\widehat{f}_1^{(freq)}(t)]$ , based of the discretization of the fluid domain  $\Omega$ ;
2. the extension of THM.4 to a generic stochastic model of the type  $\{\langle f_H \rangle, \Gamma\}$  is not possible, as proven by the subsequent discussion [see in particular THM.5].

#### 4B - Relationship between $\{f_1, \Gamma\}$ and $\{f_H, \Gamma\}$

Let us now pose the problem of determining the relationship between the 1-point PDF which characterizes the IKT statistical model  $\{f_1, \Gamma\}$  and the PDF  $f_H(t)$  associated to the statistical model  $\{f_H, \Gamma\}$ . We intend to show that  $f_1$  [with  $f_1 \equiv f_1(\mathbf{r}, \mathbf{u}, t)$ ,  $\mathbf{u} = \mathbf{v} - \mathbf{V}(\mathbf{r}, t)$  and  $\mathbf{x} = (\mathbf{r}, \mathbf{v}) \in \Gamma$ ] can be identified with a suitable stochastic-average of  $f_H$ , to be defined in terms of an appropriate nonhomogeneous and non-stationary stochastic model (see related definitions in Appendix A).

To assess properly precisely the statement let us introduce for the fluid fields  $\{Z\}$  the stochastic representation

$$\{Z(\Delta \mathbf{V})\} = \{\mathbf{V}(\mathbf{r}, t) + \Delta \mathbf{V}, p(\mathbf{r}, t)\}, \quad (58)$$

where  $\{Z\} = \{\mathbf{V}(\mathbf{r}, t), p(\mathbf{r}, t)\}$  and  $\Delta \mathbf{V} \in \mathbb{R}^3$  denote respectively an arbitrary particular solution of the INSE problem [see Appendix A] and an arbitrary velocity fluctuation. Here by assumption, the vector  $\Delta \mathbf{V} \equiv (\Delta V_1, \Delta V_2, \Delta V_3)$  will be considered as a set of stochastic hidden variables characterized by the stochastic PDF

$$g_1(\Delta \mathbf{V}, \mathbf{r}, t) \equiv f_1(\mathbf{r}, \Delta \mathbf{V}, t), \quad (59)$$

with  $f_1$  denoting the 1-point PDF characterizing the IKT statistical model  $\{f_1, \Gamma\}$  previously introduced [and obeying Eq.(9) when replacing  $\Delta \mathbf{V} \rightarrow \mathbf{v}$ ]. The set  $\{\Delta \mathbf{V}, g_1\}$  defines therefore (a generally non-homogeneous and non-stationary) stochastic model defined so that, by assumption, its moments are necessarily defined so that

$$\langle 1 \rangle_\alpha \equiv \int_{\mathbb{R}^3} d^3 \Delta \mathbf{V} f_1(\mathbf{r}, \Delta \mathbf{V}, t), \quad (60)$$

$$\mathbf{0} \equiv \int_{\mathbb{R}^3} d^3 \Delta \mathbf{V} \Delta \mathbf{V} f_1(\mathbf{r}, \Delta \mathbf{V}, t), \quad (61)$$

$$\frac{1}{2} \rho_o v_{th}^2(\mathbf{r}, t) \equiv \frac{2}{3} \rho_o \int_{\mathbb{R}^3} d^3 \Delta \mathbf{V} \frac{1}{2} (\Delta \mathbf{V})^2 f_1(\mathbf{r}, \Delta \mathbf{V}, t) \quad (62)$$

Here the moment on the r.h.s. of Eq.(62) represents, up to the constant factor  $\frac{2}{3} \rho_o$ , the stochastic mean value of the *stochastic kinetic energy per unit mass*  $\frac{1}{2} (\Delta \mathbf{V})^2$ , while  $\frac{1}{2} \rho_o v_{th}^2(\mathbf{r}, t)$  and  $v_{th}(\mathbf{r}, t)$  are the *thermal energy* and the corresponding *thermal velocity produced by the kinetic pressure*  $p_1(\mathbf{r}, t)$  [with  $p_1(\mathbf{r}, t)$  defined according to Eq. (27)]

$$v_{th}(\mathbf{r}, t) = \sqrt{\frac{2p_1(\mathbf{r}, t)}{\rho_o}}. \quad (63)$$

It follows that:

#### THM.5 - Representation of $f_1$ in terms of $f_H$

The stochastic representation (58) and position (59) can always be introduced. It follows that the stochastic

average of  $f_H$ , defined with respect to the stochastic averaging operator (106), reads identically

$$\langle f_H \rangle_{\Delta \mathbf{V}} = f_1(\mathbf{r}, \mathbf{u}, t), \quad (64)$$

with  $f_H$  given by Eq.(2).

#### PROOF

First we notice that if  $\{Z\}$  is an arbitrary particular solution of INSE, also  $\{Z(\Delta \mathbf{V})\}$  is manifestly a particular solution of the same equation. The proof is reached by introducing in the NS equation (90) [see Appendix A] a suitable stochastic volume force  $\mathbf{f} + \Delta \mathbf{f}$ , with  $\Delta \mathbf{f}$  defined so that

$$\frac{1}{\rho_o} \Delta \mathbf{f} = \Delta \mathbf{V} \cdot \nabla \mathbf{V}. \quad (65)$$

Hence, the stochastic representation (58) always holds, with  $\Delta \mathbf{V}$  to be considered as stochastic hidden variables. In addition, since the definition of  $g_1(\Delta \mathbf{V}, \mathbf{r}, t)$  is arbitrary, the position (59) can always be introduced. These definitions uniquely prescribe the stochastic model  $\{\Delta \mathbf{V}, g_1\}$  and the related stochastic averaging operator (106) [see Appendix A]. It follows that  $\langle f_H \rangle_{\Delta \mathbf{V}} \equiv \int_{\mathbb{R}^3} d^3 \Delta \mathbf{V} f_1(\mathbf{r}, \Delta \mathbf{V}, t) \delta(\mathbf{v} - \mathbf{V}(\mathbf{r}, t) - \Delta \mathbf{V})$  yields Eq.(64), which is therefore identically satisfied. Q.E.D.

In conclusion:

- the 1-point PDF of the IKT statistical model can be considered simply as a *possible stochastic realization* of the PDF  $f_H$ , achieved by means of the stochastic model  $\{\Delta \mathbf{V}, g_1\}$ , in which  $g_1$  is properly related to the 1-point PDF characterizing the IKT statistical model;
- in view of the positions (62) and (63),  $\{\Delta \mathbf{V}, g_1\}$  can be viewed as the *stochastic model which takes into account the thermal motion produced in a NS fluid by its kinetic pressure*  $p_1(\mathbf{r}, t)$  [see Eq. (27)].

#### 4C - Consequences - Statistical equation for $\langle f_1 \rangle$

The same conclusion (i.e., THM.5) holds manifestly also in the case in which the fluid fields  $\{Z\}$ , as well as the same 1-point PDF  $f_1$  and the mean-field force  $\mathbf{F}(f_1)$ , are stochastic in the sense of Eq.(13), i.e., they depend on a suitable set of stochastic hidden variables  $\alpha \in \mathbf{V}_\alpha \subseteq \mathbb{R}^n$ , here considered independent of  $\Delta \mathbf{V}$  and characterized by a stochastic PDF  $g$ . For definiteness, let us assume that  $g$  is homogeneous and stationary, i.e., of the form  $g = g(\alpha)$ . Then the ensemble average of the PDF,  $\langle f_1 \rangle$ , can be identified with

$$\langle f_1 \rangle \equiv \langle f_1 \rangle_\alpha, \quad (66)$$

with  $f_1$  defined by Eq.(64) and the brackets  $\langle \cdot \rangle_\alpha$  denoting the stochastic averaging operator (106) [Appendix A].

Hence, as a consequence of THM.5 and IKE, it follows that  $\langle f_1 \rangle$  obeys necessarily *the stochastic-averaged IKE* [14, 26]

$$\begin{aligned} \frac{\partial}{\partial t} \langle f_1 \rangle + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \langle f_1 \rangle + \frac{\partial}{\partial \mathbf{v}} \cdot \{ \langle \mathbf{F}(f_1) \rangle \langle f_1 \rangle \} &= (67) \\ = - \frac{\partial}{\partial \mathbf{v}} \cdot \{ \langle \delta \mathbf{F}(f_1) \delta f_1 \rangle \}. & \quad (68) \end{aligned}$$

Here  $\delta f_1$  and  $\delta \mathbf{F}(f_1)$  denote the stochastic fluctuations [see Eqs.(111) and (112) in Appendix A], while  $\mathbf{F}(f_1)$  is defined by Eqs. (47),(50),(51)-(53) and (38). We remark that Eq.(67) takes into account the constraints placed on  $\langle f_1 \rangle$  by the physical realizability conditions (see Section 2), as well the axioms of IKT (Section 2). Hence:

- it is appropriate for describing homogenous and stationary turbulence in NS fluids;
- however, it can be generalized, in principle, to a generally non-homogeneous and non-stationary stochastic PDF  $g$ , as appropriate for describing non-homogeneous and non-stationary turbulence [14].

The equation *departs from the statistical* (or "transport") *equation* [for  $\langle f_1 \rangle$ ] *usually considered in the literature* [see, for example, Dopazo [5] and Pope [6]]. This fact is not surprising. In fact, unlike the customary approaches, here:

- the operator of ensemble average " $\langle \rangle$ ", defined by Eqs. (64) and (66), does not commute with the relevant differential operators ( $\frac{\partial}{\partial t}, \nabla, \nabla^2$ );
- by assumption, the 1-point PDF satisfies the Liouville statistical equation defined by (9), together with the physical realizability conditions imposed on the 1-point PDF [see Eqs. (25)-(27),(17) and (20)]. These constraints are not required in the customary approach [5, 6];
- the definitions of the vector field  $\mathbf{F}(f_1)$  here adopted satisfy the requirements placed by the axiomatic formulation (see Section 2, Subsection 2A).

#### 4D - Relationship between $\{f_1, \Gamma\}$ and the HRE functional-differential approach

Finally let us consider the comparison with the HRE functional-differential approach [1, 2, 3]. In analogy to Ref.[15] let us introduce the functional

$$\phi[y(x), t] = \int_{\Gamma} d\mathbf{x} y(\mathbf{x}) f_1(\mathbf{x}, t), \quad (69)$$

which implies

$$\frac{\partial}{\partial t} \phi[y(x), t] = - \int_{\Gamma} d\mathbf{x} y(\mathbf{x}) \left[ \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} f_1(\mathbf{x}, t) + \right. \quad (70)$$

$$\left. \frac{\partial}{\partial \mathbf{v}} \cdot \{ \mathbf{F}(\mathbf{x}, t; f_1) f_1(\mathbf{x}, t) \} \right]. \quad (71)$$

Then it follows that  $\phi[y(x), t]$  must obey the following single linear functional-differential equation, manifestly equivalent to IKE (Liouville equation) (10),

$$\frac{\partial}{\partial t} \phi[y(x), t] = - \int_{\Gamma} d\mathbf{x} y(\mathbf{x}) Q \frac{\delta \phi}{\delta y(\mathbf{x})}, \quad (72)$$

where  $Q$  is related to the Liouville operator and is defined as

$$Q \cdot = \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \cdot + \frac{\partial}{\partial \mathbf{v}} \cdot \{ \mathbf{F}(\mathbf{x}, t; f_1) \cdot \}. \quad (73)$$

Eq.(72) is analogous to the Hopf  $\phi$ -equation and has the *explicit exact solution*

$$\phi[y(x), t] = \phi[T_{t_o, t} y(x_o), t_o], \quad (74)$$

where  $T_{t_o, t}$  is the evolution operator associated to the Navier-Stokes dynamical system.

#### 5 - IKT FOR MULTI-POINT PDF'S

The construction of multi-point PDF's is a problem of "practical" interest in experimental/numerical research in fluid dynamics. In fact, despite not being themselves observables, they are nevertheless related to physical observables (or conditional observables), such as the velocity difference between different fluid elements usually adopted for the statistical analysis of turbulent fluids.

In the present theory, unlike the ML approach, the statistical equation advancing in time the 1-point PDF  $f_1$  [i.e., Eq.(9)] satisfies, by definition, a kinetic closure condition. Hence, the construction of the multi-point PDF's is trivial. Nonetheless, it is still useful to analyze elementary implications (of the present theory) dealing with: a) the specific representation of certain "reduced" multi-point PDF's, defined in terms of the 1-point PDF; b) their dynamics, namely the statistical equations which they fulfill; c) their relationship with the relevant observables.

#### 5A - Liouville equations for the multi-point PDF's

Let us assume, for definiteness, that  $f_1(\mathbf{x}_i, t, \alpha; Z)$  is the 1-point PDF which is particular solution of the (1-point) Liouville equation (9). Then, denoting  $f_1(i) \equiv f_1(\mathbf{x}_i, t, \alpha; Z)$  (for  $i = 1, s$ ) the same PDF evaluated at the

states  $\mathbf{x}_i \equiv (\mathbf{r}_i, \mathbf{v}_i)$  (for  $i = 1, s$ ), the  $s$ -point PDF is the probability density

$$f_s(1, 2, \dots, s) \equiv \prod_{i=1,s} f_1(i), \quad (75)$$

defined in the product phase-space  $\Gamma^s \equiv \prod_{i=1,s} \Gamma$ . The statistical equation advancing in time  $f_s$  follows trivially from Eq.(9). In fact, denoting by  $\mathbf{F}(i) \equiv \mathbf{F}(\mathbf{x}_i, t; f_1)$  the mean-field force at the state  $\mathbf{x}_i$  (for  $i = 1, s$ ) and introducing the  $s$ -point Liouville operator (with summation understood on repeated indexes)

$$L_s(1, \dots, s) \equiv \frac{\partial}{\partial t} + \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \frac{\partial}{\partial \mathbf{r}_i} \cdot \{\mathbf{F}_i(i)\}, \quad (76)$$

it follows that  $f_s(1, 2, \dots, s)$  satisfies identically the  $s$ -point *Liouville equation* (or IKE)

$$L_s(1, \dots, s) f_s(1, 2, \dots, s) = 0. \quad (77)$$

### 5B - Consequences: reduced 2-point PDF's and 2-point observables

In terms of the 2-point PDF,  $f_2(1, 2)$ , a number of reduced probability densities can be defined in suitable subspaces of  $\Gamma^2$ . To introduce them explicitly let us first introduce the transformation to the center of mass coordinates of the two point-particles with states  $(\mathbf{r}_i, \mathbf{v}_i)$  (for  $i = 1, 2$ )

$$\{\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2\} \rightarrow \{\mathbf{r}, \mathbf{R}, \mathbf{v}, \mathbf{V}\} \quad (78)$$

[with  $\mathbf{r} = \frac{\mathbf{r}_1 - \mathbf{r}_2}{2}$ ,  $\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}$ ,  $\mathbf{v} = \frac{\mathbf{v}_1 - \mathbf{v}_2}{2}$  and  $\mathbf{V} = \frac{\mathbf{v}_1 + \mathbf{v}_2}{2}$ ]. Then, these are respectively the *local* (in configuration space) *velocity-difference 2-point PDF*:

$$g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}, t, \alpha) = \int_U d^3\mathbf{V} f_2(1, 2) \equiv \int d^3\mathbf{V} f_1(\mathbf{r}_1, \mathbf{v} + \mathbf{V}, t, \alpha) f_1(\mathbf{r}_2, \mathbf{V} - \mathbf{v}, t, \alpha; Z) \quad (79)$$

(defined in the space  $\Omega^2 \times U$ ) and the *velocity-difference 2-point PDF*, i.e., the observable

$$\hat{f}_2(\mathbf{r}, \mathbf{v}, t, \alpha) = \langle g_2(\mathbf{r} + \mathbf{R}, \mathbf{r} - \mathbf{R}, \mathbf{v}, t, \alpha) \rangle_{\mathbf{R}, \Omega} \quad (80)$$

(defined in  $\Gamma$ ),  $\langle \rangle_{\mathbf{R}, \Omega}$  denoting the configuration-space average operator acting on the center of mass. Hence, in terms of the average operator (14), there follows

$$\begin{aligned} \hat{f}_2(\mathbf{r}, \mathbf{v}, t, \alpha) &= \frac{1}{\mu(\Omega)} \int_{\Omega} d^3\mathbf{R} \\ g_2(\mathbf{r} + \mathbf{R}, \mathbf{r} - \mathbf{R}, \mathbf{v}, t, \alpha). \end{aligned} \quad (81)$$

In the case of a Gaussian PDF [(33)], Eq.(79) delivers in particular the Gaussian PDF

$$g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}, t, \alpha) = \frac{1}{\pi^{3/2} v_{th}^3} \exp \left\{ -\frac{\left\| \mathbf{v} - \frac{\mathbf{V}(1) - \mathbf{V}(2)}{2} \right\|^2}{v_{th}^2} \right\} \quad (82)$$

where  $\mathbf{V}(i) \equiv \mathbf{V}(\mathbf{r}_i, t)$ ,  $v_{th,p}^2(i) = v_{th,p}^2(\mathbf{r}_i, t)$  and  $v_{th}^2$  denotes

$$v_{th}^2 = \frac{v_{th,p}^2(1) + v_{th,p}^2(2)}{4}. \quad (83)$$

In a similar way it is possible to identify additional 2-point observables. Precisely these can be defined as:

1. *the velocity-difference 2-point PDF for parallel velocity increments.* Introducing the representations  $\mathbf{v} = \mathbf{n}v$  and  $\mathbf{r} = \mathbf{n}r$ ,  $\mathbf{n}$  denoting a unit vector,  $\hat{f}_{2\parallel}(r, v, t)$  can be simply defined as the solid-angle average

$$\hat{f}_{2\parallel}(r, v, t, \alpha) = \int d\Omega(\mathbf{n}) \hat{f}_2(\mathbf{r} = \mathbf{n}r, \mathbf{v} = \mathbf{n}v, t, \alpha); \quad (84)$$

2. *the velocity-difference 2-point PDF for perpendicular velocity increments.* Introducing, instead, the representations  $\mathbf{v} = \mathbf{n}v$  and  $\mathbf{r} = \mathbf{n} \times \mathbf{b}r$ ,  $\mathbf{n}$  and  $\mathbf{b}$  denoting two independent unit vectors,  $\hat{f}_{2\perp}(r, v, t)$  can be defined as the double-solid-angle average

$$\begin{aligned} \hat{f}_{2\perp}(r, v, t, \alpha) &= \int d\Omega(\mathbf{n}) \int d\Omega(\mathbf{b}) \\ \hat{f}_2(\mathbf{r} = \mathbf{n} \times \mathbf{b}r, \mathbf{v} = \mathbf{n}v, t, \alpha). \end{aligned} \quad (85)$$

An interesting property which emerges from these definitions is that in all cases indicated above [i.e., Eqs.(80),(84) and (85)] the definition of  $g_2$  given above [Eq.(79)] implies that non-Gaussian features, respectively in  $\hat{f}_2$ ,  $\hat{f}_{2\parallel}$  and  $\hat{f}_{2\perp}$ , may arise even if the 1-point PDF is Gaussian, i.e., the requirement (33) holds identically. This occurs due to velocity and pressure fluctuations occurring between different spatial positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . More generally, however, we can infer that - due to the constraint (17) here imposed on the 1-point PDF - it is obvious that, if the fluid velocity  $\mathbf{V}(\mathbf{r}, t)$  is bounded in the domain  $\bar{\Omega}$ , *the same 1-point PDF, and hence the 2-point PDF's, cannot be Gaussian distributions*.

### 5C - Statistical evolution equation for $\hat{f}_2$

From the 2-point IKE (77) (obtained in the case  $s = 2$ ) it is immediate to obtain the corresponding evolution equation for the reduced PDS's indicated above. For example, the velocity-difference 2-point PDF  $\hat{f}_2$  satisfies the equation

$$\begin{aligned} \frac{\partial \hat{f}_2}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \hat{f}_2 + \frac{\partial}{\partial \mathbf{v}} \cdot \frac{1}{\mu(\Omega)} \int d^3\mathbf{V} \\ \int_{\Omega} d^3\mathbf{R} \frac{\mathbf{F}_1(1) - \mathbf{F}_2(2)}{2} f_2(1, 2) = 0. \end{aligned} \quad (86)$$

It follows that, in particular, in the Gaussian case (33) this equation reduces to the (generally non-Markovian) Fokker-Planck equation

$$\frac{\partial \hat{f}_2}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \hat{f}_2 + \frac{\partial}{\partial \mathbf{v}} \cdot \frac{1}{\mu(\Omega)} \int_{\Omega} d^3 \mathbf{R} \quad (87)$$

$$\mathbf{F}^{(T)} g_2(\mathbf{r} + \mathbf{R}, \mathbf{r} - \mathbf{R}, \mathbf{v}, t, \alpha) = 0,$$

where the vector field  $\mathbf{F}_1^{(T)} \equiv \mathbf{F}_1^{(T)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{V}, t, \alpha; f_M)$  is given in Appendix C [see Eqs.(129) and 130)].

An interesting issue is provided by the comparison with the statistical formulation developed by Peinke and coworkers [34, 35, 36, 37, 38]. Their approach, based on the statistical analysis of experimental observations, indicates that in case of stationary and homogeneous turbulence both the 2-point PDF's for parallel and velocity increments obey stationary Fokker-Planck equations. In particular, according to experimental evidence [37, 38] a reasonable agreement with a Markovian approximation for Eq.(87) - at least in some limited subset of parameter space- is suggested. Our theory suggests, however, that a breakdown of the Markovian assumption should be expected due to non-local contributions appearing in the PDF's and in the corresponding statistical equations.

## 6 - DISCUSSION AND CONCLUDING REMARKS

An axiomatic approach, based on the IKT statistical model  $\{f_1, \Gamma\}$ , has been developed for the statistics of the 1-point PDF  $f_1$  which characterizes an incompressible NS fluid. The paper contains several new aspects and basic consequences of interest in fluid dynamics and turbulence theory.

Indeed, the theory here developed applies both to regular and turbulent flows, characterized respectively by deterministic and stochastic fluid fields. In fact, in both cases the time evolution of  $f_1$  is a Liouville equation (IKE) [see Eq.(9)] which evolves in time also the complete set of fluid fields (represented in terms of moments of the same PDF).

In this paper an explicit solution of the problems 1-6 posed in Subsection 1D has been proposed.

In particular, we have proven that - extending the statistical approach earlier developed [11, 12] - the IKT statistical model  $\{f_1, \Gamma\}$  can be uniquely determined. The present theory is based on two new hypotheses, i.e., A) that both  $f_1$  and  $\mathbf{F}(f_1)$  are conditional observables and B) that  $f_1$  satisfies suitable physical realizability conditions (see Subsection 2A). The first requirement permits to determine the mean-field force  $\mathbf{F}(f_1)$ , while the second one uniquely prescribes - by means of PEM (i.e., Axiom #4) - the initial PDF  $f_1(t_o)$ . In detail, we have shown that  $\{f_1, \Gamma\}$  can be constructed in such a way to be:

- unique (see THM.1, related to Problems 1);

- statistically complete (see THM.2, Problem 2);
- closed, i.e., it both moment-closure and kinetic-closure conditions (see THM.3, Problems 3 and 4)

and furthermore:

- that it determines uniquely all multi-point PDF's, as well as the related observables (see Problem 5);
- that the statistical equations for multi-point PDF's depend only on  $f_1$  and therefore, by definition, satisfy a closure condition (Problem 6).

The theory has important consequences.

First, it implies that the initial PDF is generally non-Gaussian (see again THM. 2). This conclusion holds even in the case in which the fluid fields are deterministic, namely for regular flows. In fact, the Gaussian 1-point PDF although unique (THM.1) does not generally provide a statistical complete model  $\{f_M, \Gamma\}$  (see corollary of THM.1). In addition:

- thanks to the fluid and kinetic closure conditions imposed on the statistical equation for the 1-point PDF , i.e., IKE [Eq.(9)],  $f_1$  depends only on a finite set of moments of the same PDF and its time evolution is independent of higher-order (multi-point) PDF's;
- as a basic consequence, the *exact statistical equation* for the ensemble-averaged (or stochastic-averaged) PDF  $\langle f_1 \rangle$  has been obtained. This is found to be intrinsically different from the analogous transport equation obtained in the past in the case of stationary and homogeneous turbulence [5, 6].

The connection of the present theory both with previous IKT approaches [11, 12] and the HRE (Hopf, Rosen and Edwards [1, 2, 3]) and ML (Monin and Lundgren [8, 9]) statistical treatments, has been pointed out (see, in particular, Section 4). Regarding, in particular, the last two approaches the following results have been reached:

- the common statistical model,  $\{f_H, \Gamma\}$ , used in both approaches (HRE and ML) has been shown to be generally statistically incomplete (THM.4) ;
- the relationship between the  $f_1$  and the PDF  $f_H$  which characterizes the HRE and ML approaches has been determined. In particular, we have proven that  $f_1$  can be identified with a suitable stochastic average of  $f_H$ , via a generally non-homogeneous and non-stationary stochastic PDF [see Eq.(64)];
- the unique connection [via Eqs.(64) and (66)] existing between the ensemble-averaged PDF's  $\langle f_1 \rangle$  and  $\langle f_H \rangle$  has been displayed;

- the relationship with the Hopf's functional-differential approach has been pointed out.

Finally, as an application, explicit representations have been given for the *reduced 2-point PDF's* usually adopted for the statistical description of turbulent flows, represented respectively by the velocity-difference 2-point PDF  $\hat{f}_2$  and the velocity-difference 2-point PDF for parallel and perpendicular velocity increments  $\hat{f}_{2\parallel}$  and  $\hat{f}_{2\perp}$ .

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## APPENDIX A: THE MATHEMATICAL DESCRIPTION OF INCOMPRESSIBLE NS FLUIDS

In fluid dynamics the state of an arbitrary fluid system is assumed to be defined everywhere in a suitable *extended configuration domain*  $\Omega \times I$  [ $\Omega$  denoting the configuration space and  $I \subseteq \mathbb{R}$  the time axis] by an appropriate set of suitably smooth functions  $\{Z\}$ , denoted as *fluid fields*, and by a well-posed set of PDE's, denoted as *fluid equations*, of which the former are solutions. The fluid fields are by assumption functions of the observables  $(\mathbf{r}, t)$ , with  $\mathbf{r}$  and  $t$  spanning respectively the sets  $\Omega$  and  $I$ , namely smooth real functions. Therefore, they are also *strong solutions* of the fluid equations. In particular, this means that they are required to be at least continuous in all points of the closed set  $\overline{\Omega} \times I$ , with  $\overline{\Omega} = \Omega \cup \partial\Omega$  closure of  $\Omega$ . In the remainder we shall require, for definiteness, that:

1.  $\Omega$  (*configuration domain*) is a bounded subset of the Euclidean space  $E^3$  on  $\mathbb{R}^3$ ;
2.  $I$  (*time axis*) is identified, when appropriate, either with a bounded interval, *i.e.*,  $I = ]t_0, t_1[ \subseteq \mathbb{R}$ , or with the real axis  $\mathbb{R}$ ;
3. in the open set  $\Omega \times I$  the functions  $\{Z\}$ , are assumed to be solutions of a closed set of fluid equations. In the case of an incompressible Navier-Stokes fluid the fluid fields are  $\{Z\} \equiv \{\mathbf{V}, p, S_T\}$

and their fluid equations

$$\rho = \rho_o, \quad (88)$$

$$\nabla \cdot \mathbf{V} = 0, \quad (89)$$

$$N\mathbf{V} = 0, \quad (90)$$

$$\frac{\partial}{\partial t} S_T = 0, \quad (91)$$

$$Z(\mathbf{r}, t_o) = Z_o(\mathbf{r}), \quad (92)$$

$$Z(\mathbf{r}, t)|_{\partial\Omega} = Z_w(\mathbf{r}, t)|_{\partial\Omega}, \quad (93)$$

where Eqs.(88)-(91) denote the *incompressible Navier-Stokes equations* (INSE) and Eqs. (88)-(93) the corresponding *initial-boundary value INSE problem*. In particular, Eqs. (88)- (93) are respectively the *incompressibility, isochoricity, Navier-Stokes and constant thermodynamic entropy equations* and the initial and Dirichlet boundary conditions for  $\{Z\}$ , with  $\{Z_o(\mathbf{r})\}$  and  $\{Z_w(\mathbf{r}, t)\}|_{\partial\Omega}$  suitably prescribed initial and boundary-value fluid fields, defined respectively at the initial time  $t = t_o$  and on the boundary  $\partial\Omega$ .

4. by assumption, these equations together with appropriate initial and boundary conditions are required to define a well-posed problem with unique strong solution defined everywhere in  $\Omega \times I$ .

Here the notation as follows.  $N$  is the *NS nonlinear operator*

$$N\mathbf{V} = \frac{D}{Dt}\mathbf{V} - \mathbf{F}_H, \quad (94)$$

with  $\frac{D}{Dt}\mathbf{V}$  and  $\mathbf{F}_H$  denoting respectively the *Lagrangian fluid acceleration* and the *total force per unit mass*

$$\frac{D}{Dt}\mathbf{V} = \frac{\partial}{\partial t}\mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V}, \quad (95)$$

$$\mathbf{F}_H \equiv -\frac{1}{\rho_o} \nabla p + \frac{1}{\rho_o} \mathbf{f} + \nu \nabla^2 \mathbf{V}, \quad (96)$$

while  $\rho_o > 0$  and  $\nu > 0$  are the *constant mass density* and the *constant kinematic viscosity*. In particular,  $\mathbf{f}$  is the *volume force density* acting on the fluid, namely which is assumed of the form

$$\mathbf{f} = -\nabla \phi(\mathbf{r}, t) + \mathbf{f}_R, \quad (97)$$

$\phi(\mathbf{r}, t)$  being a suitable scalar potential, so that the first two force terms [in Eq.(96)] can be represented as  $-\nabla p + \mathbf{f} = -\nabla p_r + \mathbf{f}_R$ , with

$$p_r(\mathbf{r}, t) = p(\mathbf{r}, t) - \phi(\mathbf{r}, t), \quad (98)$$

denoting the *reduced fluid pressure*. As a consequence of Eqs.(88),(89) and (90) it follows that the fluid pressure necessarily satisfies the *Poisson equation*

$$\nabla^2 p = S, \quad (99)$$

where the source term  $S$  reads

$$S = -\rho_o \nabla \cdot (\mathbf{V} \cdot \nabla \mathbf{V}) + \nabla \cdot \mathbf{f}. \quad (100)$$

### A.1 - Physical/conditional observables - Hidden variables

The fluid fields  $\{Z\}$  are, by assumption, prescribed smooth real functions of  $(\mathbf{r}, t) \in \Omega \times I$ . In particular, they can be either *physical observables* or *conditional observable*, according to the definitions indicated below.

#### *Definition - Physical observable/conditional observable*

A *physical observable* is an arbitrary real-valued and uniquely-defined smooth real function of  $(\mathbf{r}, t) \in \Omega \times I$ . Hence, as a particular case  $(\mathbf{r}, t)$  are observable too.

A *conditional observable* is, instead, an arbitrary real-valued and uniquely-defined smooth real function of  $(\mathbf{r}, t) \in \Omega \times I$  which depends also on non-observable variables and is, as such, an uniquely-prescribed function of the latter ones.

Therefore the functions  $Z_i$  can be assumed respectively of the form [13, 14]

$$Z_i \equiv Z_i(\mathbf{r}, t) \quad (101)$$

or

$$Z_i \equiv Z_i(\mathbf{r}, t, \alpha), \quad (102)$$

$\alpha \in V_\alpha \subseteq \mathbb{R}^k$  (with  $k \geq 1$ ) denoting a suitable set of *hidden variables*. In fluid dynamics these are intended as:

#### *Definition - Hidden variables*

A *hidden variable* is as an arbitrary real variable which is independent of  $(\mathbf{r}, t)$  and is not an observable.

### A.2 - Deterministic and stochastic fluid fields

Hence, fluid fields of the type (102) are manifestly non-observables. However, if in the whole set  $\overline{\Omega} \times I \times V_\alpha$ , they are uniquely-prescribed functions of  $(\mathbf{r}, t, \alpha)$  then they are *conditional observables*. Hidden variables can be considered in principle either *deterministic* or as *stochastic variables*, in the sense specified as follows.

#### *Definition - Stochastic variables*

Let  $(S, \Sigma, P)$  be a probability space; a measurable function  $\alpha : S \rightarrow V_\alpha$ , where  $V_\alpha \subseteq \mathbb{R}^k$ , is called *stochastic* (or *random*) *variable*.

A stochastic variable  $\alpha$  is called *continuous* if it is endowed with a *stochastic model*  $\{g_\alpha, V_\alpha\}$ , namely a real

function  $g_\alpha$  (called as *stochastic PDF*) defined on the set  $V_\alpha$  and such that:

- 1)  $g_\alpha$  is measurable, non-negative, and of the form

$$g_\alpha = g_\alpha(\mathbf{r}, t, \cdot); \quad (103)$$

- 2) if  $A \subseteq V_\alpha$  is an arbitrary Borelian subset of  $V_\alpha$  (written  $A \in \mathcal{B}(V_\alpha)$ ), the integral

$$P_\alpha(A) = \int_A d\mathbf{x} g_\alpha(\mathbf{r}, t, \mathbf{x}) \quad (104)$$

exists and is the probability that  $\alpha \in A$ ; in particular, since  $\alpha \in V_\alpha$ ,  $g_\alpha$  admits the normalization

$$\int_{V_\alpha} d\mathbf{x} g_\alpha(\mathbf{r}, t, \mathbf{x}) = P_\alpha(V_\alpha) = 1. \quad (105)$$

The set function  $P_\alpha : \mathcal{B}(V_\alpha) \rightarrow [0, 1]$  defined by (104) is a probability measure and is called distribution (or law) of  $\alpha$ . Consequently, if a function  $f : V_\alpha \rightarrow V_f \subseteq \mathbb{R}^m$  is measurable,  $f$  is a stochastic variable too.

Finally define the *stochastic-averaging operator*  $\langle \cdot \rangle_\alpha$  (see also [13, 14]) as

$$\langle f \rangle_\alpha = \langle f(\mathbf{y}, \cdot) \rangle_\alpha \equiv \int_{V_\alpha} d\mathbf{x} g_\alpha(\mathbf{r}, t, \mathbf{x}) f(\mathbf{y}, \mathbf{x}), \quad (106)$$

for any  $P_\alpha$ -integrable function  $f(\mathbf{y}, \cdot) : V_\alpha \rightarrow \mathbb{R}$ , where the vector  $\mathbf{y}$  is some parameter.

#### *Definition - Homogeneous, stationary stochastic model*

The stochastic model  $\{g_\alpha, V_\alpha\}$  is denoted:

- a) *homogeneous* if  $g_\alpha$  is independent of  $\mathbf{r}$ , namely

$$g_\alpha = g_\alpha(t, \cdot); \quad (107)$$

- b) *stationary* if  $g_\alpha$  is independent of  $t$ , i.e.,

$$g_\alpha = g_\alpha(\mathbf{r}, \cdot). \quad (108)$$

#### *Definition - Deterministic variables*

Instead, if  $g_\alpha(\mathbf{r}, t, \cdot)$  is a *deterministic PDF*, namely it is of the form

$$g_\alpha(\mathbf{r}, t, \mathbf{x}) = \delta^{(k)}(\mathbf{x} - \alpha_o), \quad (109)$$

$\delta^{(k)}(\mathbf{x} - \alpha_o)$  denoting the  $k$ -dimensional Dirac delta in the space  $V_\alpha$ , the hidden variables  $\alpha$  are denoted as *deterministic*.

Let us now assume that, for a suitable stochastic model  $\{g_\alpha, V_\alpha\}$ , with  $g_\alpha$  non-deterministic, the stochastic variables  $Z_i \equiv Z_i(\mathbf{r}, t, \alpha)$  and  $f_1(\mathbf{r}, \mathbf{v}, t, \alpha)$  (where  $Z_i(\mathbf{r}, t, \cdot)$

and  $f_1(\mathbf{r}, \mathbf{v}, t, \cdot)$  are measurable functions) admit everywhere in  $\overline{\Omega} \times I$  and  $\overline{\Gamma} \times I$  the *stochastic averages*  $\langle Z_i \rangle_\alpha$  and  $\langle f_1 \rangle_\alpha$  defined by (106).

Hence,  $Z_i \equiv Z_i(\mathbf{r}, t, \alpha)$ ,  $f_1(\mathbf{r}, \mathbf{v}, t, \alpha)$  and the mean-field force  $\mathbf{F}(f_1)$  [see Sections 2,3 and 4] admit also the *stochastic decompositions*

$$Z_i = \langle Z_i \rangle_\alpha + \delta Z_i, \quad (110)$$

$$f_1 = \langle f_1 \rangle_\alpha + \delta f_1, \quad (111)$$

$$\mathbf{F}(f_1) = \langle \mathbf{F}(f_1) \rangle_\alpha + \delta \mathbf{F}(f_1). \quad (112)$$

In particular, unless  $g_\alpha(\mathbf{r}, t, \cdot)$  is suitably smooth, it follows that generally  $\langle Z_i \rangle_\alpha, \delta Z_i$  and respectively  $\langle f_1 \rangle_\alpha, \delta f_1$  may belong to different functional classes with respect to the variables  $(\mathbf{r}, t)$ .

### A.3 - Deterministic and stochastic INSE problems - Regular and turbulent flows

Therefore, assuming, for definiteness, that all the fluid fields  $Z$ , the volume force  $\mathbf{f}$  and the initial and boundary conditions, are either deterministic or stochastic variables and both belong to the same functional class, i.e., are suitably smooth w.r. to  $(\mathbf{r}, t)$  and  $\alpha$ , Eqs. (88)- 93) define respectively a *deterministic* or *stochastic initial-boundary value INSE problem*. In both cases we shall assume that it admits a strong solution in  $\overline{\Omega} \times I$  (or  $\overline{\Omega} \times I \times V_\alpha$ ).

In the first case, which characterizes flows to be denoted as *regular*, the fluid fields are by assumption *physical observables*, i.e., uniquely-defined, smooth, real functions of  $(\mathbf{r}, t) \in \Omega \times I$  [with  $\Omega$ , the *configuration space*, and  $\overline{\Omega}$  its closure, to be assumed subsets of the Euclidean space on  $\mathbb{R}^3$  and  $I$ , the *time axis*, denoting a subset of  $\mathbb{R}$ ].

In the second case, characterizing instead *turbulent flows*, the fluid fields are only *conditional observables* (see again Subsection A.1). In this case, besides  $(\mathbf{r}, t)$ , they may be assumed to depend also on a suitable stochastic variable  $\alpha$ , (with  $\alpha \in V_\alpha$  and  $V_\alpha$  subset of  $\mathbb{R}^k$  with  $k \geq 1$ ). Hence they are stochastic variables too.

### APPENDIX B: DEFINITION OF $N_1$

Let us provide here an explicit definition of  $N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z)$  [required to specify also  $\widehat{f}_1^{(freq)}$  in terms of Eq.(18)]. For definiteness, let us assume that the fluid velocity is bounded, i.e., that there exists  $V_B \in \mathbb{R}$  such that in  $\Omega \times I$  for each component of the fluid velocity  $V_k(\mathbf{r}, t, \alpha)$  (with  $k = 1, 2, 3$ ) there results

$$|V_k(\mathbf{r}, t, \alpha)| \leq \frac{1}{2} V_B. \quad (113)$$

Then  $N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z)$  can be defined as follows

$$N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z) = \dots \quad (114)$$

$$= \frac{N}{c} \prod_{k=1,2,3} \Theta_{ik}(\mathbf{v}) \Theta\left(\frac{V_B^2}{4} \left[1 - \frac{1}{M}\right]^2 - v_k^2\right), \quad (115)$$

$$\Theta_{ik}(\mathbf{v}) \equiv \Theta(V_k(\mathbf{r}_i, t) - v_k - \frac{V_B}{2M}) \quad (116)$$

$$\Theta(v_k - V_k(\mathbf{r}_i, t) + \frac{V_B}{2M}),$$

with  $M \in \mathbb{N}$  and  $\Theta(x)$  the Heaviside theta function; here  $c \in \mathbb{R}$  and  $N \in \mathbb{N}$  are defined so that there results

$$c = V_B^3 \sum_{i=1,N} \prod_{k=1,2,3} \Theta_{ik}(\mathbf{v}), \quad (117)$$

$$M^3 = N. \quad (118)$$

Thanks to positions (114)-(118) for an arbitrary  $N \in \mathbb{N}$  fulfilling Eq.(118), it follows

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1,N} \int_U d^3 v N_1(\mathbf{r}_i, \mathbf{v}, t, \alpha; Z) = 1. \quad (119)$$

Hence Eq.(19) is satisfied identically.

### APPENDIX C: EVALUATION OF $\mathbf{F}^{(T)}$

In  $f_1(1)$  and  $f_1(2)$  coincide with a local Gaussian [i.e., see Eq.(33)] there results by construction

$$\int d^3 \mathbf{V} \mathbf{V} f_1(1) f_1(2) = [\beta \mathbf{v} - \mathbf{U}] f_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}; Z) \quad (120)$$

$$\int d^3 \mathbf{V} V^2 f_1(1) f_1(2) = \frac{3}{2} v_{th,p}^2 f_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}; Z), \quad (121)$$

where there results

$$\begin{aligned} \beta &= \frac{v_{th,p}^2(1) - v_{th,p}^2(2)}{v_{th,p}^2(1) + v_{th,p}^2(2)} = \\ &= \frac{1}{\frac{1}{v_{th,p}^2(2)} - \frac{1}{v_{th,p}^2(1)}}, \end{aligned} \quad (122)$$

$$\mathbf{U} = \frac{\mathbf{V}(1)v_{th,p}^2(2) + \mathbf{V}(2)v_{th,p}^2(1)}{v_{th,p}^2(1) + v_{th,p}^2(2)} = \quad (123)$$

$$= \frac{\frac{\mathbf{V}(1)}{v_{th,p}^2(1)} + \frac{\mathbf{V}(2)}{v_{th,p}^2(2)}}{\frac{1}{v_{th,p}^2(2)} - \frac{1}{v_{th,p}^2(1)}}.$$

Let us now evaluate the expression  $\int d^3 \mathbf{V} \frac{1}{2} [\mathbf{F}(1) - \mathbf{F}(2)] f_1(1) f_1(2)$ . Introducing the notations

$$\begin{aligned} \mathbf{F}_0(1) &= \frac{1}{\rho_0} \mathbf{f}(1) + [\mathbf{V} + \mathbf{v} - \mathbf{V}(1)] \cdot \nabla_1 \mathbf{V}(1) + \\ &+ \nu \nabla_1^2 \mathbf{V}(1), \end{aligned} \quad (124)$$

$$\mathbf{F}_1(1) = \frac{[\mathbf{V} + \mathbf{v} - \mathbf{V}(1)]}{2} A(1) + \quad (125)$$

$$+ \frac{v_{th,p}^2(1)}{2p_1(1)} \nabla_1 p_1(1) \left\{ \frac{[\mathbf{V} + \mathbf{v} - \mathbf{V}(1)]^2}{v_{th,p}^2(1)} - \frac{3}{2} \right\},$$

$$\mathbf{F}_0(2) = \frac{1}{\rho_0} \mathbf{f}(2) + [\mathbf{V} - \mathbf{v} - \mathbf{V}(2)] \cdot \nabla_2 \mathbf{V}(2) + \quad (126)$$

$$+ \nu \nabla_2^2 \mathbf{V}(2),$$

$$\mathbf{F}_1(2) = \frac{[\mathbf{V} - \mathbf{v} - \mathbf{V}(1)]}{2} A(2) + \quad (127)$$

$$+ \frac{v_{th,p}^2(2)}{2p_1(2)} \nabla_2 p_1(2) \left\{ \frac{[\mathbf{V} - \mathbf{v} - \mathbf{V}(2)]^2}{v_{th,p}^2(2)} - \frac{3}{2} \right\},$$

and letting for  $j = 1, 2$ ,

$$A(j) = \frac{1}{p_1(j)} \frac{D}{Dt} p_1(j) \quad (128)$$

it follows

$$\int d^3 \mathbf{V} \frac{1}{2} [\mathbf{F}(1) - \mathbf{F}(2)] f_1(1) f_1(2) =$$

$$= [\mathbf{F}_0^{(T)} + \mathbf{F}_1^{(T)}] f_2 \equiv \mathbf{F}^{(T)} f_2,$$

where

$$2\mathbf{F}_0^{(T)} = \frac{1}{\rho_0} \mathbf{f}(1) + \quad (129)$$

$$+ [(\beta + 1) \mathbf{v} - \mathbf{U} - \mathbf{V}(1)] \cdot \nabla_1 \mathbf{V}(1) +$$

$$+ \nu \nabla_1^2 \mathbf{V}(1) -$$

$$- \frac{1}{\rho_0} \mathbf{f}(2) -$$

$$- [(\beta + 1) \mathbf{v} - \mathbf{U} - \mathbf{V}(2)] \cdot \nabla_2 \mathbf{V}(2) + \nu \nabla_2^2 \mathbf{V}(2)$$

$$2\mathbf{F}_1^{(T)} = \frac{[(\beta + 1) \mathbf{v} - \mathbf{V}(1)]}{2} A(1) + \quad (130)$$

$$+ \frac{v_{th,p}^2(1)}{2p_1(1)} \nabla_1 p_1(1)$$

$$\left\{ \frac{\frac{3}{2}v_{th}^2 + 2[\beta \mathbf{v} - \mathbf{U}] \cdot [\mathbf{v} - \mathbf{V}(1)] + [\mathbf{v} - \mathbf{V}(1)]^2}{v_{th,p}^2(1)} - \frac{3}{2} \right\} -$$

$$- \frac{[(\beta + 1) \mathbf{v} - \mathbf{V}(2)]}{2} A(2) -$$

$$- \frac{v_{th,p}^2(2)}{2p_1(2)} \nabla_2 p_1(2)$$

$$\left\{ \frac{\frac{3}{2}v_{th}^2 + 2[\beta \mathbf{v} - \mathbf{U}] \cdot [\mathbf{v} - \mathbf{V}(2)] + [\mathbf{v} - \mathbf{V}(2)]^2}{v_{th,p}^2(2)} - \frac{3}{2} \right\}.$$

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